Materials Science & Technology 2004 Conference & Exhibition

SEPTEMBER 26–29, 2004
NEW ORLEANS, LOUISIANA USA

MS&T 2004

Where Theory Meets Application

MS&T '04—A CAN'T MISS EVENT

TMS and AIST Operating Committees will come together to present MS&T '04.

Where Scientists Meet Engineers

The symposia planned for MS&T '04 have been developed to present both practical and theoretical accomplishments advancing both scientific understanding and industrial progress. The complete conference consists of ferrous and nonferrous technologies, advanced and fundamental applications, proposed and hands-on processing methodologies, and a comprehensive snapshot of the present and the future for metals and materials industries.

Where Technology Meets the Future

One of the highlights of the meeting will be the extensive list of topics planned that include:

- Materials Damage Prognosis
- Pb-Free and Pb-Bearing Solders
- Titanium for Healthcare, Biomedical, and Dental Applications
- 3-Dimensional Materials Science
- Advancements in Mechanical Property Characterization at the Micro- and Nano-Scale
- Applications of Orientation Microscopy Techniques to Phase Transformation
- Continuous Casting Fundamentals
- Computational Microstructure Evolution in Steel
- Development and Application of Hot Rolled Flat Products
- Engineered Steel Surfaces
- High Strain Rate Deformation and Deformation Mechanisms of Structural Steels
- Intellectual Property Fundamentals for Materials Scientists and Managers
- Mechanical Behavior of Body-Centered-Cubic (BCC) Metals and Alloys
- Modeling and Computer Applications in Metal Casting, Shaping & Forming Processes
- Precipitation in Steels – Physical Metallurgy and Property Development
- The Effect of Primary Operations on Product Quality
- Product Application and Development
- The Accelerated Implementation of Materials & Processes
- The Effects of Microstructure and Property Homogeneity/Variability on Product Performance
- Third International Symposium on Railroad Tank Cars
- Use of Bainitic and Bainitic-Martensitic Steels in Current or Developing Applications
- Rhenium and Rhenium Containing Alloys
- Roll Technology

Where You Need to Be!

For more information on MS&T '04 or to register, visit www.matscitech.org or contact TMS Meeting Services, 184 Thorn Hill Road, Warrendale, PA 15086; Phone: 724-776-9000 ext. 243; Fax: 724-776-3770; e-mail: mtgserv@tms.org

COME SEE ALL THAT MS&T '04 HAS TO OFFER

— double the information, double the networking opportunities — for the price of a single conference. Come and join us September 26–29, 2004 in The Big Easy!

MAXIMIZE YOUR EXHIBIT INVESTMENT

MS&T '04 attendees represent leading U.S. and international corporations, world-class educational institutions, government agencies, and technical organizations. This high-level, targeted audience is actively seeking the best and most innovative technologies and solutions the industry has to offer. At MS&T '04, exhibitors can showcase their products and services, offer product demonstrations, and find the customers they are looking for — all in one place. MS&T '04 also offers a variety of marketing and sponsorship opportunities to help you enhance your presence at the conference.

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012345678

MS&T 2004

REGISTRATION FORM

Advance Registration Deadline: Tuesday, September 7, 2004.
Forms received after this date will be processed at the higher on-site fees.

AIST ASSOCIATION FOR IRON & STEEL TECHNOLOGY TMS

WEB

www.matscitech.org
Web registration requires credit card payment.

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USA: 724-776-3770
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Return with payment to:
MS&T '04
TMS
184 Thorn Hill Rd.
Warrendale, PA 15086

Member of: ☐AIST ☐TMS ☐ASM   Member Number: ____________

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Street/PO Box: ____________

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Registration Fees:	**Fees Through Sept. 7**	**Fees After Sept. 7**
☐Speaker	$425	$525
☐Member	$475	$575
☐Non-Member	$595	$695
☐Student Member*	$0	$50
☐Student Non-Member†*	$45	$95

***Registration Fee** .... **Total $**______*

† Non-member students receive membership in TMS and AIST for the calendar year 2005.

** To qualify for student rate, students must attach a copy of their student identification card.*

Speaker, member and non-member registration fees include admission to all technical sessions, the MS&T '04 CD-ROM, opening reception.

Student member and student non-member registration fees include admission to all technical sessions and the opening reception.

Publications: *ABOUT THE CD-ROM: The MS&T '04 CD-ROM contains the proceedings of selected symposia held at the conference. One copy of the CD-ROM is included in the speaker, member, and nonmember registration fees. Additional copies of the CD-ROM will be available for purchase and must be picked-up at the meeting. The MS&T '04 CD-ROM will not be available for purchase after the meeting. ABOUT THE BOOKS: All of the symposia contained on the CD-ROM are also available in printed book format in Volumes I and II, which are available for purchase at the prices listed below. Both Volumes I and II will be available at the meeting; volumes can be pre-ordered or purchased at the meeting, and shipment can be arranged for an additional fee. Both printed volumes will also be available for sale after the meeting.*

	Quantity	Member	Nonmember	Student	
MS&T '04 CD-ROM	______	$184	$266	$89	$..........

PRINT OPTION:

TITLE	**Quantity**	**Member**	**Nonmember**	**SHIIPPING U.S.**	**Can/Mex**	**Other**	
Materials Science & Technology 2004 Volume I— *Process Metallurgy, Product, Quality and Applications*	______	$95	$120	$8.00	$36.50	$56.50	$______
Materials Science & Technology 2004 Volume II*—Continuous Casting Fundamentals, Engineered Steel Surfaces, and Modeling and Computer Applications in Metal Casting, Shaping and Forming Processes*	______	$65	$85	$6.50	$23.00	$35.50	$______
2-Volume Set	______	$135	$150	$10.50	$59.00	$91.50	$______

***Publications** .... **Total $**______*

MS&T '04 Workshop: September 26

☐News Media 101 .... $289

***Continuing Education Workshop** .... **Total $**______*

Membership Dues Renewal: (For current members only.)

AIST:

☐Member* .... $95 ☐Student $52.50

TMS:

☐Full Member .... $90 ☐Junior Member $52.50

☐ASM/TMS Joint Student Member $25

***Membership Dues** .... **Total $**______*

** Includes $10 at conference discount.*

Social Function Tickets: September 27

	Fee	**Quantity**	**Total**
TMS Young Leaders Tutorial Box Lunch (*Optional*)	$35	______	$______
AIST/TMS Awards Luncheon	$45	______	$______

***Social Function Tickets** .... **Total $**______*

Foundation Contributions:

AIST: ☐$25 ☐$50 ☐Other $______

TMS: ☐$25 ☐$50 ☐Other $______

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MS&T 2004

MS&T '04 Conference Grid

	MONDAY, SEPTEMBER 27TH AM	MONDAY, SEPTEMBER 27TH PM	TUESDAY, SEPTEMBER 28TH AM	TUESDAY, SEPTEMBER 28TH PM	WEDNESDAY, SEPTEMBER 29TH AM	WEDNESDAY, SEPTEMBER 29TH PM
Grand Ballroom I			Intellectual Property Fundamentals for Materials Scientists and Managers: IP Fundamentals I: Obtaining IP Rights	Intellectual Property Fundamentals for Materials Scientists and Managers: IP Fundamentals II: Asserting IP Rights		
Grand Ballroom J		Selections From International Conference on Advanced High Strength Sheet Steels for Automotive Applications	Rhenium and Rhenium Containing Alloys: Rhenium Containing Alloys	Rhenium and Rhenium Containing Alloys: Rhenium		
Grand Ballroom K	Pb-Free and Pb-Bearing Solders: Session I	Pb-Free and Pb-Bearing Solders: Session II	Pb-Free and Pb-Bearing Solders: Session III	Pb-Free and Pb-Bearing Solders: Session IV	Pb-Free and Pb-Bearing Solders: Session V	Pb-Free and Pb-Bearing Solders: Session VI
Grand Ballroom L		High Strain Rate Deformation and Deformation Mechanisms of Structural Steels: Deformation Mechanisms and Microstructure Effects	High Strain Rate Deformation and Deformation Mechanisms of Structural Steels: Development and Application of High Strain Rate Properties	Engineered Steel Surfaces: Corrosion Protection, Coatings, Scale	Engineered Steel Surfaces: Nanotechnology, Hardness, Wear Resistance	
Grand Ballroom M		Continuous Casting Fundamentals: Initial Solidification and Interfacial Phenomena	Continuous Casting Fundamentals: Mold Fluid Flow and Water Spray Cooling	The Effects of Microstructure and Property Homogeneity/ Variability on Product Performance: Session I	The Effects of Microstructure and Property Homogeneity/ Variability on Product Performance: Session II	
La Galerie 1	Roll Technology: Practices Affecting Rolls	Roll Technology: Cold and Hot Mill Rolls	Roll Technology: Maintenance and Inspection	Primary Operations and Product Quality: Session I		Materials and Critical Societal Issues Special Session:
La Galerie 2		Modeling & Computer Applications in Metal Casting, Shaping & Forming Processes: Modeling & Computer Simulation: Tube Making & Related Processes	Modeling & Computer Applications in Metal Casting, Shaping & Forming Processes: Modeling & Computer Simulation: Thermal Treatment & Related Processes	Modeling & Computer Applications in Metal Casting, Shaping & Forming Processes: Modeling & Computer Applications: Casting Processes	Modeling & Computer Applications in Metal Casting, Shaping & Forming Processes: Modeling & Computer Applications: Shaping & Rolling Processes	
La Galerie 3	Precipitation in Steels - Physical Metallurgy and Property Development: HSLA Steels: Microalloying	Precipitation in Steels - Physical Metallurgy and Property Development: Phase Transformation	Precipitation in Steels - Physical Metallurgy and Property Development: HSLA Steels: Cu-, Cr-Precipitation	Precipitation in Steels - Physical Metallurgy and Property Development: Precipitation in High Alloyed Steels	Development and Application of Hot Rolled Flat Products: Session I	
La Galerie 4	Computational Microstructure Evolution in Steel: Computational Microstructure Evolution	Computational Microstructure Evolution in Steel: Stress, Strain and Deformed Microstructures	Computational Microstructure Evolution in Steel: Recrystallization and Grain Growth	Computational Microstructure Evolution in Steel: Multiphase Microstructure Evolution		

MS&T '04 Conference Grid

Room	MONDAY, SEPTEMBER 27TH AM	MONDAY, SEPTEMBER 27TH PM	TUESDAY, SEPTEMBER 28TH AM	TUESDAY, SEPTEMBER 28TH PM	WEDNESDAY, SEPTEMBER 29TH AM	WEDNESDAY, SEPTEMBER 29TH PM
La Galerie 5	Product Application and Development: Session I	Product Application and Development: Session II	Product Application and Development: Session III	Materials Damage Prognosis: Probabilistics, Risk, and Uncertainty Methods I	Materials Damage Prognosis: Local & Global Methods & Sensors for Interrogation of Materials Damage State I	
La Galerie 6	Materials Damage Prognosis: Overviews and Applications	Materials Damage Prognosis: Integrated Health Management	Materials Damage Prognosis: Multi-Scale Modeling and Simulation	Materials Damage Prognosis: Probabilistics, Risk, and Uncertainty Methods II	Materials Damage Prognosis: Local & Global Methods & Sensors for Interrogation of Materials Damage State II	Materials Damage Prognosis: Materials Failure and Signature Analysis
Mardi Gras Ballroom A	General Abstracts: Development & Characterization of Alloys, Nano Materials and Bulk Amorphous Metals	General Abstracts: Mechanical Behavior & Characterization	General Abstracts: Processing and Process Modeling	Mechanical Behavior of Body-Centered-Cubic (BCC) Metals and Alloys: Dynamic Behaviors	Mechanical Behavior of Body-Centered-Cubic (BCC) Metals and Alloys: Yielding and Plastic Flow	Mechanical Behavior of Body-Centered-Cubic (BCC) Metals and Alloys: Texture, Radiation, and Solute Effects
Mardi Gras Ballroom B	Third International Symposium on Railroad Tank Cars: Session I	Third International Symposium on Railroad Tank Cars: Session II	Advancements in Mechl. Property Characterization at the Micro- & Nano-Scale: Dvlp. & Application of Mechanical Property Characterization Methods I	Advancements in Mechl. Property Characterization at the Micro- & Nano-Scale: Dvlp. & Application of Mechanical Property Characterization Methods II	Advancements in Mechl. Property Characterization at the Micro- & Nano-Scale: Modlg., Simulation, & Experiml. Observa-tions of Dimensional Size Effects	Advancements in Mechanical Property Characterization at the Micro- and Nano-Scale: Application of Nanoindentation Methods
Mardi Gras Ballroom C		Use of Bainitic and Bainitic-Martensitic Steels in Current or Developing Applica-tions	Applications of Orientation Micros-copy Techniques to Phase Transformations: Ferrous Alloys I	Applications of Orientation Micros-copy Techniques to Phase Transformations: Ferrous Alloys II	Applications of Orientation Micros-copy Techniques to Phase Transformations: Emerging Techniques and Applications	Applications of Orientation Micros-copy Techniques to Phase Transformations: Nonferrous Alloys
Mardi Gras Ballroom D	All Conference Plenary	Titanium for Healthcare, Biomedi-cal, and Dental Applications: Beta Titanium Alloys	Titanium for Healthcare, Biomedi-cal, and Dental Applications: Fatigue and Wear	Titanium for Healthcare, Biomedi-cal, and Dental Applications: Processing	Titanium for Healthcare, Biomedi-cal, and Dental Applications: Composites and Coatings	Titanium for Healthcare, Biomedi-cal, and Dental Applications: Dental Applications and Phase Transformations-Microstructure
Mardi Gras Ballroom F/G	3-Dimensional Materials Science: Serial Sectioning I	3-Dimensional Materials Science: Serial Sectioning II	3-Dimensional Materials Science: X-Ray Techniques	3-Dimensional Materials Science: 3D Atom Probe/ Computational Methods I	3-Dimensional Materials Science: Computational Methods II	3-Dimensional Materials Science: Mathematical Representation
Mardi Gras Ballroom H	The Accelerated Implementation of Materials & Processes: Overviews	The Accelerated Implementation of Materials & Processes: Mechanical Properties - Titanium	The Accelerated Implementation of Materials & Processes: The Design-Materials Interface: Closing the Loop	The Accelerated Implementation of Matls. & Processes: Microstructure Modlg.: 1st Principle Theory, Phase Field & Thermo-dynamic Modeling	The Accelerated Implementation of Materials & Processes: Mechanical Property Modeling - Superalloys	

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MS&T '04 Technical Program

TOUR REGISTRATION FORM

DEADLINE: ***THURSDAY, AUGUST 26, 2004.***

PRE-REGISTRATION FORM
DESTINATION MANAGEMENT, INC. NEW ORLEANS
Has Arranged Tours for Attendees of:
MS&T '04

Please make your reservation by noting choice of tour, day, and time.
All day tours will depart from the Hyatt Regency, New Orleans

Tour Date/Tour Description	*Tour Time*	*Price*	*No. of Tickets*	*Amount Due*
Monday, September 27, 2004				
A Ride on the Wild Side Tour	8:00am – 12:00pm	$55		
Tuesday, September 28, 2004				
Jean Lafitte Swamp Tour	8:00am – 12:00pm	$39		
Haunted History Tour	6:30pm – 9:00pm	$40		
Wednesday, September 29, 2004				
Laura Plantation Tour	8:30am – 12:00pm	$27		

Once you have made your reservation and your payment has been processed, you will receive a confirmation via regular mail at least 30 days prior to your tour. If you do not receive a confirmation, please call 800/471-8222 extension 1715 to verify that DMI has received you registration form. (NO PHONE ORDERS WILL BE ACCEPTED)

Please note that you can log onto the MS&T '04 website to view the tours avaialble and register for the tours online.

Please make checks payable to and mail to:
DESTINATION MANAGEMENT, INC. NEW ORLEANS
610 South Peters Street, Suite 200 · New Orleans, Louisiana 70130
----- Attention: Ashley Dorris -----
Credit card orders may be faxed to 504/592-0529

Please fill out all information below using the names of the person(s) attending the tours.

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Address:	
City, State & Zip:	
Email Address:	
Telephone:	
Fax Number:	
Payment Options: (US Funds Only)	☐ Charge My Acct. ☐ MC ☐ Visa ☐ American Express ☐ Discover ☐ Check Enclosed

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*If your credit card information is not correct or if your card expires within two weeks, your payment may not be processed correctly and you will not be registered for the tour. In the event your credit card does not process, we will attempt to contact you only two times before we void the registration form.

TOUR REGISTRATION WILL NOT BE ACCEPTED BY PHONE. Please have your reservations in by August 27, 2004. Cancellations must be received in writing by August 27, 2004. You will receive a full refund for any cancellations received by this date. Tour is based on 35 participants. DMI reserves the right to cancel any tours should the minimum number not be met in which case refunds for all reservations will be given. The Minerals, Metals and Materials Society has the option to guarantee the minimum number of tours and pay the difference between the guaranteed number and the amount of participants. Tours are not cancelled and refunds are not given due to inclement weather. DMI acts only as an agent of suppliers when securing transportation, accommodations, and other services, and is not responsible for any delay, error or omission, loss or accident, faults or negligence of hotels, bus companies, airlines and other suppliers. Accordingly, participants agree to seek remedies directly with suppliers and not to hold DMI liable, in the absence of its negligence, for loss, injury, delay, or substitution of similar accommodations or services to the participants. If you have any questions regarding your tour registration please call Ashley Dorris a 800/471-8222 extension 1715.

All Conference Plenary

Sponsored by: AIST, TMS
Program Organizer: E. Buddy Damm, The Timken Company, Canton, OH 44706-0930 USA

Monday AM Room: Mardi Gras Ballroom D
September 27, 2004 Location: Marriott New Orleans Hotel

8:30 AM Plenary
Creating Customer Value - A Prescription for the Steel Industry: *James W. Griffith*[1]; [1]The Timken Company, Canton, OH 44706 USA

Don't call 911. The patient is the U.S. steel industry and it's in critical condition. We're familiar with the obvious symptoms (structural excess capacity, low cost imports, legacy costs, etc.) of an industry in crisis. Underlying these symptoms is a more serious disease; the loss of market share due to the substitution of other materials such as plastics or aluminum. Curing the ills of the steel industry will involve a complex treatment, one that must include the development of products that create real customer value. But don't call 911. Call the customer instead.

9:15 AM Break

3-Dimensional Materials Science: Serial Sectioning I

Sponsored by: TMS - Structural Materials Division
Program Organizers: Marc J. De Graef, Carnegie Mellon University, Department Material Science & Engineering, Pittsburgh, PA 15213-3890 USA; Jeff P. Simmons, Air Force Research Laboratory, Materials & Manufacturing Directorate, Dayton, OH 45433 USA; George Spanos, Naval Research Laboratory, Physical Metallurgy Branch, Washington, DC 20375-5000 USA; Jonathan E. Spowart, UES Inc., Dayton, OH 45432 USA

Monday AM Room: Mardi Gras Ballroom F/G
September 27, 2004 Location: Marriott New Orleans Hotel

Session Chairs: Jonathan Spowart, UES Inc., Wright-Patterson AFB, OH 45433 USA; George Spanos, Naval Research Laboratory, Washington, DC 20375-5000 USA

9:30 AM Invited
Three-Dimensional (3D) Microstructure Visualization and Finite Element Modeling of the Deformation Behavior of Metal Matrix Composites: *V. V. Ganesh*[1]; N. Chawla[1]; [1]Arizona State University, Dept. of Chem. & Matls. Engrg., Ira A. Fulton Sch. of Engrg., Tempe, AZ 85287-6006 USA

The mechanical behavior of particle reinforced metal matrix composites is significantly affected by reinforcement particle size, shape, morphology and distribution. In this study, a serial sectioning process was developed to reconstruct the three-dimensional microstructure of silicon carbide particle reinforced aluminum composite. The reconstructed 3D microstructure was used to visualize the spatial arrangement of reinforcement particles in the composite. The 3D microstructure was then incorporated into a finite element model to simulate the uniaxial deformation behavior of the composite. Comparisons between the 3D microstructure-based FEM model with idealized unit cell models, and 2D microstructure based models were conducted. It will be shown that the 3D microstructure-based model provided the closest agreement to the experimental data. The advantages of the 3D microstructure-based FEM approach, as well as some limitations, will be discussed.

10:00 AM Break

10:30 AM
Tomographic Spectral Imaging: Comprehensive 3D Microanalysis: *Paul G. Kotula*[1]; Michael R. Keenan[1]; Joseph R. Michael[1]; [1]Sandia National Laboratories, Matls. Characterization Dept., PO Box 5800, MS 0886, Albuquerque, NM 87185-0886 USA

A methodology is described for comprehensive 3D x-ray microanalysis in a dual-beam FIB/SEM (FEI Co. DB-235). In brief, the FIB is used to serially section a site-specific region of a sample and then the electron beam is rastered over the exposed surfaces with x-ray spectral images being acquired at each section. All this is performed without rotating or tilting the specimen between FIB cutting and SEM imaging/x-ray spectral image acquisition. The resultant 4D spectral image is then unfolded (number of volume elements by number of channels) and subjected to the same multivariate curve resolution (MCR) approach[1] that has proven successful for the analysis of lower-dimension x-ray spectral images. [1]P.G. Kotula, M.R. Keenan, and J.R. Michael, Microsc. Microanal. 9 (2003) 1-17. [2]Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United Stated Department of Energy (DOE) under contract DE-AC0494AL85000.

10:50 AM
Three-Dimensional Aspects of Morphological and Crystallographic Selection in Primary Si Growth for Near-Eutectic Al-Si Alloys: *Choonho Jung*[1]; Emrah Simsek[2]; Ralph E. Napolitano[1]; [1]Iowa State University, Dept. of Matls. Sci. & Engrg., 204A Wilhelm Hall, Ames, IA 50010 USA; [2]Ames Laboratory, Materials & Engineering Physics, 116 Wilhelm Hall, Ames, Iowa 50010 USA

Three-dimensional aspects of morphological evolution and selection of crystallographic texture in the angular primary silicon phase is investigated for near-eutectic alloys. Angular silicon "plate-dendrites" are grown directionally in a Bridgman-type furnace at velocities in the regime of 10^{-3} m/sec. Serial milling and x-ray techniques are combined with backscattered electron diffraction analysis to examine the early-stage selection mechanisms and the complex twinned structure of the "dendrite" cores in the steady-state microstructure. The role of twinning in the mechanisms of branching and morphological selection are discussed. The overall growth kinetics are examined with regard to diffusive transport, primary spacing, and primary growth front morphology.

11:10 AM
3D Microstructural Characterization of Carbide Distributions in Superalloys: *Robert Williams*[1]; Gopal B. Viswanathan[1]; James L. Larsen[2]; Hamish L. Fraser[1]; [1]Ohio State University, Matls. Sci. & Engrg., 477 Watts Hall, 2041 College Rd., Columbus, OH 43210 USA; [2]Air Force Research Laboratory, Matls. & Mfg. Direct., Wright-Patterson AFB, OH 45433 USA

Various types of interstitial elements (e.g., C and B), which form complex carbides, are added intentionally as these particles contribute significantly to property enhancement. The importance of these carbides in providing sufficient creep and fatigue resistance is however dependent on the size, shape and the distribution of these in the microstructure. Hence it is important to study these various features when effecting an alloy development program.; traditional techniques for materials characterization rely on the transition from 2-D sections to 3-D representations using stereology. In this study, new techniques for characterizing directly 3-D microstructures have been applied to the case of the carbide distribution in the microstructures of two Ni-base superalloys, i.e. IN100 and Waspalloy. Several series of images (as a function of depth) of the microstructure in these alloys were obtained by serial sectioning using a focused ion beam (FIB) in an FEI DB235 workstation. The 3D reconstructed image obtained from these experiments clearly shows that in the case of Waspalloy the carbides were present mostly on the grain boundaries and subgrain boundaries whereas in the case of IN100 alloy, in addition to the grain boundary carbides, blocky carbides were also seen inside the gains. The size, shape and distribution of these carbides have been obtained and analyzed. The techniques involving the serial sectioning procedures and 3D image reconstruction methods will be discussed in detail in the context of carbide distribution in these alloys. The authors are grateful for the support of the Air Force Research Laboratory and the Air Force Office of Scientific Research (Dr. Craig Hartley as Program Manager) under the STW-21 program.

11:30 AM Invited
3D Characterization of the Structure and Crystallography of Aerospace Materials Using a Dual FIB Microscope: *Michael D. Uchic*[1]; Michael Groeber[2]; Robert Wheeler[3]; Frank Scheltens[3]; Dennis M. Dimiduk[1]; [1]Air Force Research Laboratory, Matls. & Mfg. Direct., AFRL/MLLMD, 2230 Tenth St., Wright-Patterson AFB, Area B, Dayton, OH 45433 USA; [2]Ohio State University, Dept. of Matls. Sci. & Engrg., Columbus, OH 43210 USA; [3]UES, Inc., 4401 Dayton-Xenia Rd., Dayton, OH 45432 USA

The Dual Beam Focused Ion Beam (FIB)-Scanning Electron Microscope (SEM) has proved to be a powerful instrument for characterizing the microstructure and crystallography of aerospace materials in 3D. The DB FIB-SEM is capable of in-situ, high fidelity serial sectioning, where the serial sectioning slice thickness can be less than 100 nanometers, and the interrogated volume can be as large as 50 x 50 x 50 micrometers in dimension. Custom software scripts have been developed at AFRL to automate the serial sectioning experiments. The scripts are designed to acquire a variety of characterization data for each section, which can include electron images, ion images, crystallographic orientation maps (EBSD), and chemistry maps (EDS). This talk will focus on the application of the Dual Beam microscope to characterize powder metallurgy Ni base superalloys in 3D, but examples from other alloy systems will also be shown. Selected aspects of post-processing of the 3D serial sectioning data, segmentation routines for semi-automated identification of selected microconstituents, 3D reconstruction results, and preliminary analysis of micro-constituents in 2D and 3D are discussed from the view of work in progress.

Computational Microstructure Evolution in Steel: Computational Microstructure Evolution

Sponsored by: TMS - Structural Materials Division, TMS - EMPMD/ SMD-Chemistry & Physics of Materials Committee, TMS - MPMD-Computational Materials Science & Engineering-(Jt. ASM-MSCTS)
Program Organizers: Koenraad G.F. Janssens, Sandia National Laboratories, Materials and Process Modeling, Albuquerque, NM 87185-1411 USA; Mark T. Lusk, Colorado School of Mines, Mechanical Engineering Program, Division of Engineering, Golden, CO 80401 USA

Monday AM — Room: La Galerie 4
September 27, 2004 — Location: Marriott New Orleans Hotel

Session Chair: Koenraad G.F. Janssens, Sandia National Laboratories, Albuquerque, NM 87185 USA

9:30 AM Plenary
Physically-Based Large-Scale Texture and Anisotropy Simulation for Automotive Sheet Forming: *Dierk Raabe*[1]; Franz Roters[1]; [1]Max Planck Institute for Iron Research, Max-Planck-Str. 1, Duesseldorf D-40237 Germany

Abstract not available.

10:30 AM
Microstructure Modeling for Advanced High Strength Steels: *Matthias Militzer*[1]; [1]University of British Columbia, Ctr. for Metallurgl. Process Engrg., Vancouver, BC V6T 1Z4 Canada

Modeling the microstructure evolution, in particular the austenite-ferrite phase transformation, is crucial for advanced high strength steels with multi-phase microstructures. Traditionally, macroscopic, semi-empirical approaches are employed for transformation models e.g. based on the Johnson-Mehl-Avrami-Kolmogorov (JMAK) theory. However, a more rigorous approach is necessary to enhance the predictive capabilities. On the continuum scale, a phenomenological mixed-mode model is proposed where the underlying diffusion and interface mechanisms are considered in detail. However, interfacial parameters are currently not independently known such that they have to be concluded from overall transformation data. Atomistic modeling appears to be a promising approach to obtain separate information on these parameters. Further, macroscopic models do not predict the size and spatial distributions of the transformation products. This information can be obtained with modeling on the meso-scale, e.g. by using the phase field approach. The challenges of the proposed computational approaches will be evaluated for dual-phase steels.

10:50 AM
Study and Modeling the Kinetics of Bainite Formation in TRIP Steels: *Fateh Fazeli*[1]; Matthias Militzer[1]; [1]University of British Columbia, Ctr. for Metallurgl. Process Engrg., 309-6350 Stores Rd., Vancouver, BC V6T1Z4 Canada

The predictive capabilities of the existing modeling approaches for the bainite reaction, i.e. Johnson-Mehl-Avrami-Kolmogorov, diffusion and displacive methodologies, are examined. Employing these modeling philosophies to analyze the measured kinetics, a thorough comparison of the different models is provided and potential limitations of the existing models are delineated. The experimental transformation results were quantified for isothermal bainite formation in the range of 350 to 450°C for model 0.18C-1.55Mn-1.7Si and Fe-0.6C-1.5Mn-1.5Si TRIP steels. Austenite embedded in the ferrite matrix and single austenite have been adopted as initial parent phase, for the low- and high-carbon steels, respectively. The challenges will be discussed to replicate the bainite formation kinetics in TRIP steels from a fundamental point of view for a wide range of investigated temperatures where different bainite morphologies have been detected.

11:10 AM
Theory and Simulation of Microstructural Evolution: *Kegang Wang*[1]; Martin E. Glicksman[1]; Krishna Rajan[1]; [1]Rensselaer Polytechnic Institute, Matls. Sci. & Engrg., 110 8th St., Troy 12180 USA

Microstructural evolution is very common processes in phase transformation of materials. It remains as an active and important topic in materials science. Classical theory, as formulated by Lifshitz and Slyozov and by Wagner (LSW), excludes all interactions among coarsening particles and ignores local environmental information. LSW coarsening rate and particle size distribution, however, differ markedly from experimental results. In order to study the case of non-zero volume fraction, we proposed screening theory that includes interaction among particles. To simulate the dynamics of phase coarsening we formulated and solved multiparticle diffusion equations, including both interactions among particles and the influence of local environments, or "locales." Our simulations also reveal that the growth rates of individual particles deviate nonlinearly from the LSW predictions with increasing volume fraction. Fluctuations are described using "multiplicative noise." Finally, we developed more comprehensive stochastic theory for microstructural evolution.

11:30 AM Break

11:50 AM Invited
Commercial Applications of Heat Treat Simulations: Current Practice and Future Directions: *B. Lynn Ferguson*[1]; [1]Deformation Control Technology, Inc., 7261 Engle Rd., Ste. 105, Cleveland, OH 44130 USA

Abstract not available.

12:30 PM
Helium and Hydrogen Clustering in Radiation Damaged Iron Studied by Stochastic Simulations: *Chaitanya S. Deo*[1]; S. G. Srivilliputhur[1]; Michael I. Baskes[1]; Stuart Maloy[1]; Michael R. James[2]; [1]Los Alamos National Laboratory, MST-8, PO Box 1663, MS G755, Los Alamos, NM 87545 USA; [2]Los Alamos National Laboratory, D-5, PO Box 1663, MS K575, Los Alamos, NM 87545 USA

Micro-structural defects are introduced in materials upon irradiation with energetic particles. These defects can cause degradation of mechanical properties and contribute to material failure. Transmutation products such as hydrogen and helium in irradiated stainless steels exert deleterious effects on material properties. A description of the atomic mechanisms governing the process and their correlation to material properties will result in better understanding of the mechanisms by which iron and iron-based alloys respond to helium and hydrogen implantation by radiation and will suggest methods of alloy improvement to withstand irradiation damage. We have performed kinetic Monte Carlo (KMC) simulations of point defect diffusion and clustering in bcc alpha iron. The model consists of the following entities in bcc iron: interstitial and substitutional helium and hydrogen atoms, interstitial iron atoms, vacancies, vacancy-clusters, and sinks for the trapping of point defects (dislocations and grain boundaries). Input to the simulations includes the migration energies of the point defects (interstitial iron, vacancy, interstitial and substitutional helium and hydrogen), formation energies of the HenVm clusters, dissociation energies of the point defects from the HenVm clusters and initial concentrations and configurations of point defects and defect ratios. These quantities are obtained from experimental data, molecular dynamics (MD) simulations using embedded atom and modified embedded atom potentials. The defect ratios and configurations can obtained from the post-cascade data of large MD runs. We employ the KMC simulations to investigate the time evolution of the point defect configuration leading to defect clustering and bubble formation. The composition of embryonic defect clusters as a function of time and operating temperatures is determined.

12:50 PM
Combined Probability Distributions of Random-Walks: A New Method to Simulate Diffusion Processes: *Henrik Larsson*[1]; John Ågren[1]; [1]Royal Institute of Technology, Dept. Matl. Sci. Engrg., Stockholm SE-100 44 Sweden

In this talk a new technique to simulate diffusion processes will be presented. The technique is based upon conceiving diffusion as a random-walk process and utilises the probability distributions of the walks to calculate the temporal evolution of the composition profiles. The diffusion problem is solved directly in the lattice fixed frame of reference allowing a straightforward calculation of the Kirkendall effect. Furthermore, when simulating diffusion controlled phase transformations, it is not necessary to impose any special condition at the interfaces, such as local equilibrium.

1:10 PM
Computational Estimation of Heat Transfer Curves for Microstructure Prediction and Decision Support: *Aparna S. Varde*[1]; Elke A. Rundensteiner[1]; Mohammed Maniruzzaman[2]; *Richard D. Sisson*[2]; [1]Worcester Polytechnic Institute, Dept. of Computer Sci., 100 Inst. Rd., Worcester,

MA 01609 USA; [2]Worcester Polytechnic Institute, Ctr. for Heat Treating Excellence, 100 Inst. Rd., Worcester, MA 01609 USA

Experimental data in quenching heat treatment is used to plot cooling curves and heat transfer coefficient curves that serve as good visual tools to characterize the results of experiments. Since performing a real experiment consumes time and resources, it is desirable to estimate these curves computationally, given experimental conditions. At CHTE-WPI, a technique called AutoDomainMine is being proposed that performs this estimation. This helps users determine various tendencies from the estimated curve, useful in the heat treating industry. Earlier work at CHTE-WPI, namely QuenchMiner, predicts certain output parameters given quenching experimental conditions, thereby helping in decision support about materials selection. However the parameters predicted are mostly textual or numeric such as cooling uniformity and ranges of cooling rates. AutoDomainMine estimates the actual curves obtained as a result of quenching, thus assisting in even more accurate prediction of required parameters, hence further enhancing decision support. Also, an important goal in heat treating is prediction of microstructure at different points on a cooling curve. This is done in QuenchMiner by superimposing the cooling curve over Jominy End Quench results. AutoDomainMine assists in microstructure prediction by estimating the cooling curve required for this superimposition. The design of AutoDomainMine is a topic of ongoing research. This technique proposes to combine the knowledge of a domain expert with the mathematical and statistical approach provided by data mining methods, to learn the criteria for performing an accurate estimation. Data mining is the process of discovering interesting patterns in existing data sets in order to guide decisions about future activities. The proposed technique is a form of domain-type-depdendent data mining. AutoDomainMine is expected to achieve a considerably high level of accuracy and efficiency in estimating cooling curves/heat transfer coefficient curves given quenching experimental conditions. It thus provides useful information for microstructure prediction and decision support.

General Abstracts: Development & Characterization of Alloys, Nano Materials and Bulk Amorphous Metals

Sponsored by: AIST, TMS

Program Organizers: Dennis M. Dimiduk, Air Force Research Laboratory, Materials & Manufacturing Directorate, WPAFB, OH 45433 USA; E. Buddy Damm, The Timken Company, Canton, OH 44706-0930 USA; James C. Foley, Los Alamos National Laboratory, Los Alamos, NM 87545 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Monday AM — Room: Mardi Gras Ballroom A
September 27, 2004 — Location: Marriott New Orleans Hotel

Session Chair: James C. Foley, Los Alamos National Laboratory, Los Alamos, NM 87545 USA

9:30 AM
Characterization of Inert Gas Atomized Metallic Glass Powders: *Frank Biancaniello*[1]; Laszlo Kecskes[2]; Steven Mates[1]; Stephen Ridder[1]; [1]NIST, 100 Bureau Dr., Stop 8556, Gaithersburg, MD 20899-8556 USA; [2]US Army Research Laboratory, AMSRD-ARL-WM-MD, B4600, Aberdeen Proving Ground, MD 21005-5069 USA

Glass forming metal alloy powder was produced in a small, 100 g to 250 g, laboratory-scale inert gas atomizer. Results on two glasses are reported: a binary Cu-Zr composition, with a poor glass forming ability, and a quinary Hf-Nb-Cu-Ni-Al composition, with a significantly more robust glass forming ability. The powder yield from each atomization run was classified into 10 μm- sized intervals and was subsequently analyzed for crystalline content using x-ray diffraction and scanning electron microscopy. Regardless of the initial oxygen content of the parent ingot, particles < 45 μm appeared to be fully X ray amorphous. Microhardness measurements were used in conjunction with the X ray analysis to estimate Young's modulus, identify the primary crystallization species, and understand the effect of key atomization parameters on the amorphous-to-crystalline transition for each composition.

9:50 AM
Intermediate-Range Order of Ni-Based Ternary Amorphous Metals: *Michelle L. Tokarz*[1]; [1]University of Michigan, Ctr. for Nanomatls. Sci., 3062 H.H. Dow Bldg., Matls. Sci. & Engrg. Dept., Ann Arbor, MI 48109-2136 USA

Traditional X-ray experiments determined Radial Distribution Functions (RDFs) of NixNbySn100-x-y bulk amorphous alloys found a divergence from a random hard-sphere model with respect to neighbor shell distances/coordination numbers. However, these functions do not provide information about the specific contributions of any individual element. Solving the Partial Pair Distribution Functions (PPDFs) by varying the composition, or by chemical substitution, assumes similar behavior in different chemical environments, which may not be the case. Anomalous x-ray scattering provides better way to probe the local interactions of specific chemical pairs. Data near and far from the absorption edges of individual elements gives Differential Distribution Functions (DDFs), revealing the atomic arrangements. High-resolution synchrotron anomalous scattering experiments have indicated Ni-based clustering effects. This non-random distribution of atomic species may partially explain the failure of the random model. An analysis is given in terms of the short and intermediate range order of this series. Research supported by DARPA under contract number: DAAD19-01-1-0525 via a subcontract from California Institute of Technology, and by DOE for use of the synchrotron facilities the Stanford Synchrotron Radiation Laboratories.

10:10 AM
Structure of Quaternary Ni60(NbxTa100-x)34Sn6 Alloys: *Michelle L. Tokarz*[1]; [1]University of Michigan, Ctr. for Nanomatls. Sci., 3062 H.H. Dow Bldg., Matls. Sci. & Engrg. Dept., Ann Arbor, MI 48109-2136 USA

A series of alloys of nominal composition Ni60(NbxTa100-x)34Sn6 were studied using high resolution synchrotron scattering methods on beamline 2-1 at Stanford Synchrotron Laboratory. The results are compared with traditional laboratory x-ray experiments. These alloys showed mixed nanocrystalline/amorphous character over the whole range of compositions that were explored. Analysis of the diffraction patterns using standard state baselines via NIST LaB6 specimens permitted detailed determinations of the crystalline/amorphous ratios. Observations of line broadening of crystalline contributions enabled grain size distributions to be determined. Finally long-term temperature stability measurements in the vicinity of Tg showed that these alloys were more stable than the ternary Ni-based bulk metallic glasses. The stability of the amorphous/crystalline microstructure has potential to be exploited as an in situ nanocomposite. Research supported by DARPA under contract number: DAAD19-01-1-0525 via a subcontract from California Institute of Technology, and by DOE for use of the synchrotron facilities the Stanford Synchrotron Radiation Laboratories.

10:30 AM
Preparation and Microstructure Characterization of ZnO Nanocrystals: Yinghong Xiao[1]; Hongbo Liu[1]; Xiaoheng Liu[1]; Lude Lu[1]; Xin Wang[1]; [1]Nanjing University of Science and Technology, Dept. of Matls. Sci. & Tech., #200, Xiaolingwei, Nanjing, Jiangsu 210014 China

Anisotropy inherence is a crucial factor in determining the shape of nanocrystals, and is affected by the controlled external conditions. Shape-controlled ZnO nanocrystals were synthesized in Ethylene Glycol (EG) and water mixture using zinc acetate dihydrate as the starting material. By changing the temperature and the adding ways of water, sphere-, cone- and teardrop-shaped ZnO nanocrystals were obtained. The structure and morphology of the obtained powder was characterized by means of XRD and TEM. The obtained ZnO crystals were either aggregated spheres or irregular shaped. It is considered that the coordination number of Zn^{2+} kept four in the hydrolysis reaction and the growth unit of a crystal was composed of coordination tetrahedron. ZnO is a compound semiconductor with a wide and direct band gap of 3.3 eV. The calculated band gap increased with the reaction time and temperature, which corresponded to the decrease of ZnO nanocrystal size. Effect of surfactants on reaction was also investigated. Addition of PVP to the reaction system could obviously retard the reaction process due to its coordination with Zn^{2+}.

10:50 AM Break

11:00 AM
Analysis of Diffusion Couples in Multicomponent Systems: *M. A. Dayananda*[1]; L. R. Ram-Mohan[2]; [1]Purdue University, Sch. of Matls. Engrg., 501 Northwestern Ave., W. Lafayette, IN 47907 USA; [2]Quantum Semiconductor Algorithms, Inc., 5 Hawthorne Cir., Northborough, MA 01532 USA

MultiDiFlux is a user-friendly, educational, and research computer program being developed to aid in interdiffusion calculations from a single diffusion couple in binary and ternary systems. The program fits the experimental data for concentration profiles by cubic Hermite interpolation polynomials, calculates the locations of the Matano plane for the individual components and then evaluates the profiles of interdiffusion fluxes for all components directly from the smoothened concentration profiles. From appropriate integrations of the flux profiles based on Dayananda's analysis, the MultiDiFlux program calculates the ternary interdiffusion coefficients over various, selected concentration ranges within the diffusion zone of the couple. These coefficients are then utilized to generate the concentration profiles of the couples on the basis of error function solutions appropriate for the selected concentration ranges. The details of the code are presented and discussed with application to diffusion couples in selected binary and ternary systems. This research is supported by the National Science Foundation.

11:20 AM

Preparation and Annealing Behavior of Ultrafine Grain Magnesium Alloy AZ31: *Qi Yang*[1]; Amit K. Ghosh[1]; [1]University of Michigan, Matls. Sci. & Engrg., 2300 Hayward St., Ann Arbor, MI 48109 USA

Ultrafine grain microstructures can be created by the accumulation of large plastic strains, and recovery and recrystallization of the deformed structures. The size and stability of such structures have large effects on strength and formability in metallic alloys. Control of the uniformity of grain structures has been found to be a problem, which requires innovative processing approaches. In this work, a surface-shear based deformation processing, called MCF [Multipass Coining (or Corrugating) and Flattening], has been employed step-by-step to impart very large plastic strain to Mg-3%Al-1%Zn magnesium alloy billet. Deformation processing has been carried out in the temperature range of 120-250°C in an effort to obtain a uniformly submicrocrystalline grain structure in this alloy. The microstructural evolution during post-deformation static annealing at different temperatures is being examined to determine the stability of this MCF processed alloy in terms of grain growth and textural change. (Research project is sponsored by National Science Foundation Award DMR 0314218.)

11:40 AM

Properties of Ceramic Mold and Mechanical Properties of Open Cell Al Foam: *Bo-Young Hur*[1]; Bu-Keoun Park[1]; Yong-Su Um[1]; [1]Gyeongsang National University, ULSFoM-NRL, ReCAPT, Dept. of Metallurgl. & Matls. Engrg., Chinju 660-701 S. Korea

The various manufacturing processes are classified according to the state of matter in which the metal is processed solid, liquid, gaseous or ionised. Liquid metal can be foamed directly by injecting gas or gas-releasing blowing agents, or by producing supersaturated metal-gas solutions. Indirect methods include investment casting, the use of space holding filler materials or melting of powder compacts which contain a blowing agent. The purpose of this paper is to study mixture ceramic mold which can be easily removed and withstand casting temperature and pressure for investment casting method. The results of thermal expansion measure is show the fact that mixture ceramic mold shrunk at 140, 380, and 500°C. The burnout strength of mixtures ceramic mold is decrease with temperature increasing. The burnout strength of ceramic mold is ranges from 1.2 to 2.5kgf/cm^2. Open cell Al is fabricated by using mixture ceramic mold. Investigated mechanical properties of open cell Al foam with hypoeutectic and eutectic Al-Si alloy.

12:00 PM

Factors Influencing the Modification of Hypereutectic Al-Si Alloys for Production of High Integrity Automotive Pistons: *Shahrooz Nafisi*[1]; *Reza Ghomashchi*[1]; Jalal Hedjazi[2]; S. M.A Boutorabi[2]; [1]University of Quebec, Dept. of Applied Scis., 555 Univ. Blvd., Chicoutimi, Quebec G7H-2B1 Canada; [2]Iran University of Science and Technology, Metl. Dept., Narmak, Tehran Iran

Al-Si hypereutectic alloys are widely used in auto-industry for applications where wear resistance is of prime concern. . Furthermore, their low thermal expansion coefficient, and high strength to weight ratio make them the chosen material for fabrication of automotive pistons and engine blocks. Although the primary silicon particles impart adequate wear resistance, but the alloy full potential would only be realized if silicon morphology, size and distribution are optimized and closely controlled. Furthermore, the machining of hypereutectic alloys would be a tool intensive operation if the primary silicon particles are not well distributed and sized. Therefore, the addition of minor amounts of P and/or Sr may be the solution to optimize the primary and eutectic silicon particles within hypereutectic Al-Si alloys. The effects of Cu-P15% and Al-Sr10% master alloys as strong modifiers have been investigated on the microstructure of Hypereutectic Al-Si (17-19) % alloys. Thermal analysis has been employed to examine the morphological changes of Si particles and identify the optimum concentration of P and Sr to achieve a fine and well distributed silicon, i.e. eutectic and primary. The results have shown that the temperature for silicon nucleation, and the liquidus and solidification temperature range are the important parameters in understanding the refining process.

Materials Damage Prognosis: Overviews and Applications

Sponsored by: TMS - Structural Materials Division

Program Organizers: James M. Larsen, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson AFB, OH 45433-7817 USA; Jeffrey R. Calcaterra, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson Air Force Base, OH 45433-7817 USA; Leo Christodoulou, Defense Advanced Research Agency, Arlington, VA 22203-1714 USA; Michael L. Dent, Anteon Corporation USA; William J. Hardman, Naval Air Systems Command, Propulsion and Power Directorate (AIR 4.4.2), Patuxent River, MD 20670-1534 USA; Paul Hoffman, United States Navy, NAVAIR, Patuxent River, MD 20670 USA; J. Wayne Jones, University of Michigan, College of Engineering, Department of Materials, Science and Engineering, Ann Arbor, MI 48109 USA; Stephan M. Russ, Air Force Research Laboratory, Materials and Manufacturing Directorate, AFRL/MLLN, Wright-Patterson Air Force Base, OH 45433-7817 USA

Monday AM — Room: La Galerie 6
September 27, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Leo Christodoulou, Defense Advanced Research Projects Agency, Arlington, VA 22203-1714 USA; James M. Larsen, Air Force Research Laboratory, Metals, Wright-Patterson AFB, OH 45433-7818 USA

9:30 AM Invited

Materials Damage Prognosis - A Revolution in Asset Management: *Leo Christodoulou*[1]; James M. Larsen[2]; [1]Defense Advanced Research Projects Agency, DSO, Arlington, VA 22203-1714 USA; [2]Air Force Research Laboratory, Wright Patterson AFB, OH 45433 USA

Materials damage prognosis involves the integration of three key technologies: (i) real-time in situ interrogation of the materials damage state, (ii) physics-based models of the life-limiting damage processes and (iii) automated reasoning to combine all available information on the past and present state of the structural systems or subsystems, and to make a robust prediction of the future capability of the system. This presentation will highlight novel methods, both local and global, for interrogating materials to determine their intrinsic behavior and then linking this signature to physics-based multi-scale models that predict damage accumulation in materials and the cascading effect on future performance. The problem of prediction is made tractable by constraining the predictions to the short term. Examples are presented of the benefits of prognosis for real-time asset management, long-term sustainment, and initial design of highly robust systems that take full advantage of the prognosis concept.

10:00 AM Invited

Integrated Prognostic System of Systems Health Management: *Douglas E. Adams*[1]; Mark J. Smith[1]; Alok Chaturvedi[1]; Mario Rotea[1]; Christoph Hoffmann[1]; Bruce Craig[1]; [1]Purdue University, Sch. of Mechl. Engrg., Ray W. Herrick Labs., 140 S. Intramural Dr., W. Lafayette, IN 47907-2031 USA

An overview of multi-disciplinary research needs and approaches for managing the health of Systems of Systems (SOSs) is provided. SOSs are sets of interconnected systems that once operated independently but have become interdependent due to revolutionary changes in demand, competition (military and otherwise) and technology. Prognosis is an assessment of capability that is made continuously as SOSs evolve and is the key to integrated health management. SOS applications to be discussed include air/sea/land vehicle fleets in the U.S. Air Force, Navy and Army; commercial and public transportation networks; electrical power distribution grids; and commercial and defense product manufacturing chains. Fundamental research themes include 1) hierarchical modeling of physical and human systems, 2) intelligent information gathering and management, 3) continuous simulation and experimentation, 4) prediction and 5) decision-making. The focus of the talk is on developing foresight for SOS to anticipate emergent failures in capability. To this end, prognosis tools and methods are used to produce capability reports that generate and simulate worst-case scenarios. Several hypothetical examples of integrated prognostic SOSs health management are described.

10:25 AM Invited

Engine System Prognosis: *Matthew B. Buczek*[1]; Jerrol W. Littles[2]; [1]GE Aircraft Engines, Matls. & Process Engrg., 1 Neumann Way, MD H-85, Cincinnati, OH 45215 USA; [2]Pratt & Whitney, Matls. & Processes Engrg., 400 Main St., MS 114-43, E. Hartford, CT 06108 USA

Prognosis will revolutionize the way military engines are managed in the field. Instead of lifing parts to hard time limits the commander will have the ability to adaptively manage these assets to their full capability.

This will provide significant improvements in safety, readiness, and cost of ownership. GE Aircraft Engines and Pratt & Whitney have teamed in a DARPA/DSO sponsored effort make this a reality. A modular approach is being used which assesses the remaining life, and associated prediction uncertainty, for the key engine subsystems. This is accomplished by sensing the current state of the critical parts/subsystems and using physically based models to predict remaining life. A novel system architecture is used to reason between various sensed inputs and engine parameter evidentiary information. This paper provides the blueprint for Engine System Prognosis. Along with this, areas of particular technical challenge are identified.

10:50 AM Break

11:05 AM Invited
Structural Integrity Prognosis System: *John M. Papazian*[1]; Elias Anagnostou[1]; Stephen Engel[1]; John Madsen[1]; Robert Silberstein[1]; James Whiteside[1]; [1]Northrop Grumman Integrated Systems, Airborne Early Warning & Elect. Warfare, Bethpage, NY 11714 USA

As part of the DARPA Prognosis Program, we are developing a science-based approach to the prediction of the structural integrity of DoD vehicles. The work is motivated by the need for more efficient use of expensive assets and for enhanced combat readiness of critical vehicles. The Structural Integrity Prognosis System (SIPS) will provide prompt, informed predictions of the structural viability of individual assets based on tracking of their actual use and modeling of anticipated usage. The prognosis system will be founded on a collaboration between sensor systems, advanced reasoning methods for data fusion and signal interpretation, and modeling and simulation systems. Modeling and simulation will use physics-based models that faithfully capture the microstructural basis of damage mechanisms and rely on knowledge of the actual material microstructures. A variety of sensor systems will be employed, including global and local devices, and their output will be translated into state awareness by suitable algorithms. Uncertainties in the sensor and modeling data will be evaluated and codified by the reasoning and prediction system. Demonstrations of the applicability of the system to aircraft and rotorcraft structures and to rotorcraft power trains are planned.

11:30 AM Invited
Structural Prognosis: What Everyone Should Know!: *Paul C. Hoffman*[1]; [1]United States Navy, NAVAIR Struct. Div., Code 4.3.3, Patuxent River, MD 20670-1906 USA

During the Cold War Era, end of service life of a military air platform was predicated on aircraft performance obsolescence not on an airframe fatigue life limit. Things have changed! We need to adopt a structural prognosis perspective that reflects the reality of the expectant life of airframes and attendant structural integrity risks. For military aircraft, the major structural disease is fatigue. The development is the accumulation of load cycles with the inevitable outcome being end of structural service life. The prediction of end of service life is the prognostic challenge. The challenge has us asking the question of what is it we should know to be able to predict. We will define what constitutes a cogent prognosis system. Consequently we will be cognizant of what information should be collected to provide input.

Pb-Free and Pb-Bearing Solders: Session I

Sponsored by: TMS - Electronic, Magnetic & Photonic Materials Division, TMS - EMPMD-Electronic Packaging and Interconnection Materials Committee
Program Organizers: C. Robert Kao, National Central University, Department of Chemical and Materials Engineering, Chungli City 32054 Taiwan; W. Plumbridge, Open University, School of Engineering Materials, Milton Keynes MK7 6AA UK; K. N. Subramanian, Michigan State University, Chemical Engineering & Material Science, East Lansing, MI 48824 USA

Monday AM — Room: Grand Ballroom K
September 27, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: K. N. Subramanian, Michigan State University, Dept. of Chem. Engrg. & Matls. Sci., E. Lansing, MI 48824 USA; Jin Yu, Korea Advanced Institute of Science & Technology, Ctr. for Elect. Pkgg. Matls., Daejon 305-701 Korea

9:30 AM Opening Remarks

9:35 AM Invited
Creep Behavior of Sn-Ag Solder: *James C.M. Li*[1]; Fuqian Yang[2]; [1]University of Rochester, Dept. of Mechl. Engrg., Rochester, NY 14627 USA; [2]University of Kentucky, Dept. of Chem. & Matls. Engrg., Lexington, KY 40506 USA

Impression Creep Properties of Sn3.5Ag was studied in the temperature range of 333 to 453 K and punching stress range of 3.5-60 MPa. The stress dependence of impression rate is found to obey a hyperbolic sine function of stress. Based on such stress dependence a single activation energy of 51 kJ/mole can describe the temperature dependence of creep rate in the whole range. The propopsed creep mechanism is that of grain boundary fluid flow similar to the case of Pb-Sn eutectic alloy in which the interfacial fluid flow is the controlling mechanism. This analysis appears better than the power law analysis of stress dependence and the use of many mechanisms in different stress and temperature regions. This work was partially supported by NSF through a grant DMR-0211706 monitored by Drs. Guebre Tessema and Bruce A. MacDonald.

10:05 AM
Impression Creep Studies on Dispersion Strengthened Sn-Ag and Sn-Ag-Cu: *Pranesh Aswath*[1]; Aravind Munukutla[1]; Purushotham Kaushik[1]; [1]University of Texas, Matls. Sci. & Engrg. Program, 500 W. First St., Rm. 325, Arlington, TX 76019 USA

Lead free solders are slated to replace lead bearing solders in the near future as a result of the proposed legislation banning lead in electronic assemblies. However, the mechanical reliability aspects of these solders are still not as well documented as their lead bearing counterpart. Previously several investigators have studied the creep behavior of these solders using bulk samples but in the current investigation, Impression creep testing has been performed on solders comparable in size and morphology found in a typical board level interconnect structure. Activation energy and stress exponent have been determined for Sn-Ag, Sn-Ag-Cu and their Ag and Cu dispersion strengthened counterparts. In addition, the effect and interactions of dwell time/reflow time, cooling rate, base alloy, dispersion material and Percentage reinforcement on the creep strain rate have been evaluated using both OFAT (One Factor at A Time) and DOE (Design of Experiments) based testing.

10:30 AM
Creep Deformation of Sn-Rich Solder Joints: *S. B. Kim*[1]; Jin Yu[1]; T. Y. Lee[2]; [1]Korea Advanced Institute of Science and Technology, Ctr. for Elect. Pkgg. Matls., 373-1, Kusong-dong, Yusong-Gu, Daejon 305-701 Korea; [2]Hanbat National University, Dept. of Matl. Engrg., 16-1, San, Dukmyoung-Dong, Yusong-Gu, Daejon 305-719 Korea

Creep properties of Sn & Sn-0.7Cu based alloy which contained Bi, Sb, Zn or Bi were studied by single lapshear creep test. Solder balls with 8 different compositions of Sn-x & Sn-0.7Cu-x (x=0.5Bi, 0.5Sb, 0.5Zn and 0.5In) were reflowed on Ni-P pad. The Ni3Sn4 intermetallic compound(IMC) formed between Sn-x solders and Ni-P substrate, while the Cu6Sn5 IMC formed between Sn-0.7Cu-x and Ni-P. Sn-0.7Cu-x alloys showed better creep resistance than Sn-x alloys because Cu6Sn5 particles were dispersed in the solder matrix.

10:55 AM
Processing and Creep Properties of Ag and Al2O3 Reinforced Sn-Cu Based Composite Solder Joints: *Fu Guo*[1]; Feng Tai[1]; Jianping Liu[1]; Yanfu Yan[1]; Yaowu Shhi[1]; [1]Beijing University of Technology, Coll. of Matls. Sci. & Engrg., 100 Ping Le Yuan, Chaoyang Dist., Beijing 100022 China

Composite approach has been effective in providing lead-free solder joint with such enhanced mechanical properties as tensile strength, creep resistance, and thermomechanical fatigue resistance. Choices of appropriate inert reinforcements tend to minimize grain boundary sliding/decohesion so as to homogenize the solder joint deformation and thus improve the service capability of the solder joint. Sn-Cu based composite solder joints were prepared with mechanically incorporated micron-sized Ag and Al2O3 reinforcements. Processing properties in terms of wetting characteristics of the composite solders were evaluated for various Ag and Al2O3 volume fractions. Creep rupture life and creep rates of the composite solder joints were quantified and compared with their non-composite counterparts. Creep deformation features were observed and corresponding mechanisms were analyzed.

11:20 AM
Developments in COST 531 (Lead-Free Solder Materials): *William John Plumbridge*[1]; [1]Open University, Walton Hall, Milton Keynes MK76AA UK

This European programme was established to develop second generation solder alloy systems, working from thermodynamic principles. Working Groups have been set up covering the basic sciences, materials properties, performance and packaging. In addition, several specific Projects, involving participation of laboratories from different countries, have been designed. The presentation will outline the nature and progress of these investigations as at September 2004.

Precipitation in Steels - Physical Metallurgy and Property Development: HSLA Steels: Microalloying

Sponsored by: AIST, AIST - Division V, AIST - Division VI
Program Organizers: Luis Ruiz-Aparicio, Duferco Farrell Corporation, Farrell, PA 16121 USA; Dengqi Bai, IPSCO Inc., Muscatine, IA 52761 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Monday AM Room: La Galerie 3
September 27, 2004 Location: Marriott New Orleans Hotel

Session Chair: Luis J. Ruiz-Aparicio, Duferco Farrell Corporation, Quality & Process Tech., Farrell, PA 16121 USA

9:30 AM Invited
Precipitation Hardening of Ferrite in Commercially Processed Niobium-Bearing HSLA Steels: *Anthony J. DeArdo*[1]; William Kepler Whiteford[1]; [1]University of Pittsburgh, Basic Metals Procg. Rsch. Inst., Dept. of Matls. Sci. & Engrg., Pittsburgh, PA USA

It has been known for over 60 years that the addition of small amounts of niobium to HSLA steels can result in dramatic increases in strength. For over 40 years, these additions, in combination with proper hot processing and cooling have also been associated with dramatically improved toughness, as well. The increase in strength found with Nb additions has often been attributed to precipitation hardening of the ferrite by small particles of NbC or NbCN. There is no shortage of TEM micrographs in the literature allegedly supporting this view. Quantitative analysis of the evidence however does not support the view that precipitation hardening of ferrite by NbC ever exceeds about 80-100MPa. This paper will review the precipitation reactions in ferrite and the resulting dispersions of precipitates. These will be compared to the dispersions required by Orowan- Ashby for various levels of precipitation hardening. Evidence will be presented to show that when Nb additions lead to large increases in strength, the conditions under which it does so also promote different types of ferrite. Hence, the real strengthening effect is one of dislocation or subgrain boundary hardening and not precipitation hardening.

10:05 AM
Transformation and Precipitation Behavior in Low-Carbon Microalloyed Steels: *Toyohisa Shinmiya*[1]; Nobuyuki Ishikawa[1]; Shigeru Endo[1]; [1]JFE Steel Corporation, Steel Rsch. Lab., 1 kokan-cho, Fukuyama, Hiroshima prf. 721-8510 Japan

Thermomechanical controlled processing (TMCP) is applied to manufacturing high strength steel plates. In this study, transformation and precipitation behavior of low carbon microalloyed steels in various TMCP conditions, such as quenching and tempering (Q+T) and accelerated cooling (AcC), was investigated. Microstructures were bainite and cementite in all conditions, but cementite morphology was different, which was related to bainite transformation or tempering conditions. In Q+T steel, large amount of nano-meter sized precipitates, which were NaCl type complex carbonitride consisted of Nb, Mo and Ti mainly, were formed. It was found that these precipitates were thermally stable at tempering temperature and the morphology did not change during heat treatment. Effects of tempering conditions, such as temperature, heating rate and holding time, on cementite morphology and precipitation behavior will be discussed.

10:30 AM
Control of Grain Size by Second Phase Particle Additions in Novel HSLA Strips: *Cheng Ai Khoo*[1]; George Fourlaris[1]; [1]University of Wales, Matls. Rsch. Ctr., Singleton Park, Swansea SA2 8PP UK

High Strength Low Alloy (HSLA) strip steels have extensive applications in the automotive industry, due to their excellent combination of strength, toughness and formability characteristics. The purpose of the present study is to study the control of austenite grain size via second phase particle additions, based on combined titanium and vanadium microalloy additions. Processing of HSLA strips steels aims to produce a fine austenite grain size resulting in the subsequent formation of a fine primarily ferritic product. Two experimental titanium and titanium-vanadium HSLA grades were studied, as part of this comparative study. The present study confirmed that vanadium carbide precipitates succesfully control the austenite grain size at low austenitisation temperatures (900-950°C), by effectively pinning the austenite grain boundaries. However, at higher austenitisation temperatures (in excess of 1000°C) rapid dissolution of vanadium carbide does occur and the importance of titanium nitride formation in controlling the austenite grain size, in both experimental grades, becomes evident.

10:55 AM Break

11:05 AM
Microstructural Evolution During Run-Out Table Cooling of Niobium Bearing HSLA Strip Steels: *Ian Paul Barnard*[1]; Georgios Fourlaris[1]; [1]University of Wales, Matls. Rsch. Ctr., Swansea SA2 8PP UK

HSLA steels possess a combination of high strength and ductility, properties that are imparted through the addition of microalloying additions of elements such as niobium, titanium and vanadium. HSLA steels are used widely in in the manufacturing industry as a result of these unique properties attained following controlled hot rolling and accelerated cooling. This processing route controls the strengthening mechanisms such as phase transformation, precipitation hardening and grain refinement. The present study is concerned with the effect of varying controlled cooling conditions on the run-out table on precipitation in Nb-HSLA strip steel. Using the Gleeble 3500 thermomechanical simulation unit the hot rolling process is being simulated with particular emphasis upon the run-out table cooling. Characteristics of the hot-rolling process being investigated are the finishing temperature, the coiling temperature and the cooling rate between these two temperatures. Additionally, the effect of variable nitrogen contents on the precipitation reactions and microstructural evolution of Nb-HSLA strip steels is also studied.

11:30 AM
Characterisation and Modelling of NbC Heterogeneous Precipitation in Model IF Steels: *Fabien Perrard*[1]; Alexis Deschamps[1]; Patricia Donnadieu[1]; Philippe Maugis[2]; [1]Domaine Universitaire, LTPCM-ENSEEG, Groupe Physique du Metal, BP 75, Saint Martin d'Heres 38402 France; [2]IRSID-Arcelor, Voie Romaine, BP 30320, Maizieres les Metz 57283 France

Precipitation of NbC in low carbon steels is of large practical interest, however no detailed quantitative characterisation of the precipitation kinetics is available. In this study, precipitation kinetics in ferrite are investigated for two model Fe-Nb-C alloys containing respectively 400 and 790 ppm of Nb and 58 and 110 ppm of C. The volume fraction and precipitate size are followed by Small-Angle Neutron Scattering (SANS) measurements. Precipitate morphology and location are determined by Transmission Electron Microscopy (TEM) observations. TEM observations show that precipitates form mainly on dislocations and with a regular spacing. SANS results demonstrate that both alloys show very similar precipitation kinetics, due to the heterogeneous precipitation process. Transition from dislocation-controlled to volume-controlled coarsening is observed. A precipitation model is developed which describes the role of dislocations as preferential nucleation sites and short-circuit diffusion paths. This model is successfully applied for both alloys over a range of three temperatures.

11:55 AM
Hot Deformation Behavior of Mn-Al and Mn-Al-Nb Steels: *E. Poliak*[1]; F. Siciliano[1]; N. Fonstein[1]; D. Bhattacharya[1]; T. Carneiro[2]; [1]Ispat Inland Inc., 3001 E. Columbus Dr., E. Chicago, IN 46312 USA; [2]R&D Reference Metals Company Inc.

Effects of high Al content (up to 1.7 wt. %) on high temperature dynamic and static restoration in austenite with • 1.5 - 1.8% % Mn and its interaction with NbC precipitation in microalloyed steels are studied in laboratory hot compression simulations. Along with strengthening at increasing Al and/or Nb content, simulations reveal abnormal variations in the peak and steady state strains, as well as in critical strains for initiation of dynamic recrystallization and strain hardening rate. To explain these abnormalities, it is assumed that Al in combination with Mn creates nonhomogeneous distribution of carbon in austenite at the temperatures typical for hot forming. This can result in non-uniform deformation resistance in austenite and induce additional strain gradients that can facilitate recrystallization and lead to abnormalities in peak strains. In Nb microalloyed steels this can be further accompanied by non-uniform precipitation in austenite predominantly in carbon enriched zones.

Product Application and Development: Session I

Sponsored by: AIST, AIST - Division VI
Program Organizers: E. Buddy Damm, The Timken Company, Canton, OH 44706-0930 USA; Amy Bailey, TXI - Chaparral Steel, Midlothian, TX 76065 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Monday AM — Room: La Galerie 5
September 27, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Amy J. Bailey, TXI - Chaparral Steel, Process Metall. - Bar Mill, Midlothian, TX 76065 USA; Brian Nelson, Dofasco Inc., Hamilton, ON L8N 3J5 Canada

9:30 AM
Successful Product Development: *Pete Jarocewicz*[1]; Vicky Weddington[1]; Jeffery Luksa[1]; [1]The Timken Company, Application Dvlp. - Steel, 1835 Dueber Ave. SW, PO Box 6930, Canton, OH 44706 USA

The need to be responsive to product development demands in the market place is critical in today's competitive environment. Successful product development requires a comprehensive process and the necessary resources to provide a technically comprehensive solution in a timely manner. This includes a systemic approach to the gathering, evaluation, and management of development opportunities. These projects can be as simple as a slight change in chemical composition for improved mechanical properties and part performance. Projects can be as complex as a joint effort between a customer, academia, and the supplier to design and develop a new grade and process for an application. This presentation will outline the process utilized at the Timken Company to achieve successful product development. Included will be examples of product development projects cutting across various industries such as communications (materials for broadcast tower support structures), automotive (forged crankshaft development), and energy (a down hole oil well application).

9:55 AM To Be Announced
Abstract not available.

10:20 AM
Partnership in Development and Application of Technologies: Praxair and Usiminas Experience in Installations of Cojet System in the BOF: *Ismar Antonio Sardinha*[1]; Ricardo Bastos dos Santos[1]; Luis Octavio Barros de Souza[1]; [1]Praxair Metals Technologies, Rua Cristiano F.T. Guimaraes - 50, Contagem, MS 32010-130 Brasil

Major changes in the iron and steel industry over the past several years have forced companies to look for viable ways to stay competitive. Technology is recognized as a key element to be competitive and comes from successfully linking, development, and management of ideas from engineering, marketing, and production centers. In 2002, a relationship was formed between Praxair and USIMINAS to utilize each company's varied background, experience, and knowledge to implement and refine a new technology. From this partnership, advancements in the application of the Cojet Gas Injection System in the Basic Oxygen Furnace have been forged. This paper will discuss the model developed by Praxair and USIMINAS in the use of the Cojet System in BOF applications and the model´s success in creating a mutual competitive advantage.

10:45 AM Break

11:05 AM
Controlled Thermo-Mechanical Processing of Tube and Pipe for Enhanced Manufacturing and Performance: Robert V. Kolarik[1]; *Craig V. Darragh*[1]; Jeffery E. Ives[1]; Daqing Jin[1]; E. Buddy Damm[1]; Michael E. Burnett[1]; [1]The Timken Company, 1835 Dueber Ave., MC RES - 4, PO Box 6930, Canton, OH 44706 USA

Steel seamless mechanical tubing is used in many engineered applications including as a feedstock for the manufacture of precision bearings and gears. The concept advanced in the Controlled Thermo-Mechanical Processing project done at The Timken Company is that the behavior of steel tube or pipe product can be well enough understood or characterized to suggest a preferred or optimum microstructure for an intended application. The CTMP concept continues with the assertion that by combining the knowledge of metallurgical, thermal and deformation fundamentals, the steps in the tube-making process can be adequately represented in a model to predict the product microstructure. The concept concludes with the idea that such a model can be used by someone with the process expertise to develop a recipe for the best manufacturing path for a given product order. A Tube Optimization Model (TOM) has been built by Timken under a partial funding award from the U.S. Department of Energy. The TOM has been used in conjunction with predictive and performance tests to develop recipes for tube processing that enhance manufacturing and reduce processing cost.

11:30 AM
Heavy Wall Induction Bends for the Offshore Industry: *Firdosh H. Kavarana*[1]; [1]Shaw NAPTech, Inc., Tech. Serv. Div., 210E, 700S, Clearfield, UT 84015 USA

Shaw NAPTech, Inc, a member of The Shaw Group Inc., is a pioneer in the production of heavy wall, high yield induction bends for critical service in the offshore industry. For the first time these induction bends were made from a micro alloyed grade X-65/70 seamless line pipe steel with wall thickness up to 2? and diameter up to 13?. These induction bends were installed at a depth of upto 6000 feet below water and at operating pressures of 15,000 psi. The proper chemistry was formulated to obtain the required strength and toughness properties in these heavy wall pipe bends from the thermomechanical control processing adopted during the induction bending process. Following induction bending an optimum tempering process was adopted to take advantage of the various precipitation reactions occuring in these kind of alloys. Extensive microstructural characterizations, fracture toughness testing and corrosion testing affecting material properties were carried out.

11:55 AM
Development of Co-Extruded, Oxide Dispersion Strengthened Tubes for Ethylene Pyrolysis: *Marvin G. McKimpson*[1]; Matthew T. King[1]; [1]Michigan Technological University, Inst. of Matls. Procg., 1400 Townsend Dr., Houghton, MI 49931 USA

A program has been undertaken to develop high performance tubes for production of ethylene and other industrial chemicals. These wrought tubes consist of an inner core of Incoloy® alloy MA 956 surrounded by an outer sheath of a mechanically alloyed, oxide dispersion strengthened (ODS) variant of Alloy 803 (36Fe-35Ni-27Cr + Al, Ti, Si, Mn, C). They are produced by direct powder extrusion of the ODS Alloy 803 around a thick-walled, tubular preform of Incoloy® alloy MA 956. The program involves development of the ODS Alloy 803 alloy, finite element modeling of the co-extrusion process, production of the clad tubes, and laboratory-scale evaluation of these tubes to assess coking, joining and elevated temperature characteristics. The results of this development program will be reviewed. Work sponsored by the Office of Industrial Technologies, U.S. Department of Energy under contract DE-FC36-01ID14255.

Roll Technology: Practices Affecting Rolls

Sponsored by: AIST, AIST - Division V
Program Organizers: Ron Webber, Dofasco Inc., Hamilton, Ontario L9G 4T1 Canada; Phil Perry, NSC/PMD Nippon Steel, Plant & Machinery Division, Crown Point, IN 46307 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Monday AM — Room: La Galerie 1
September 27, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Phil Everman, Nucor Steel, Hickman, Armorel, AR 72310 USA; Manfred Haissig, MH Consulting, Harrisburg, NC 28075 USA

9:30 AM
The Optimization of FM Work Roll Cooling Condition for HSM: *Wang Changan*[1]; Fei Yi Ruo[2]; [1]Baosteel, Hot Rolling Mill Plant, Shanghai 200941 China; [2]Baosteel, Admin., Fujin Rd., Baoshan, Shanghai 201900 China

In combination with the experience to expand the usage of HSS work roll in a hot mill, the paper tried to sort out the key elements which influence the roll-cooling effect, hence the roll performance; quantitatively analyzed the elements by means of painted roll and roll simulator. The optimization work was done according to the analysis. The optimization work had good effect on roll-out-of-mill temperature, roll surface, the HSS roll use and roll cost.

9:55 AM
Modelling of Thermal Mode and Calculation of Coolant System of Mill: *E. A. Garber*[1]; A. I. Vinogradov[1]; A. I. Traino[1]; V. S. Yusupov[1]; [1]Russian Academy of Sciences, A.A. Baikov Inst. of Metall., 49, Leninsky pr, Moscow 119991 Moscow

During hot rolling of especially thin strips of a thickness of 1.0-1.2 mm, a roll-coolant system does not cope with a tap in heat. Therefore, creation of a technique of industrial auditing of coolant systems of broad-strip mills for the definition of the parameters of their redesign is an actual problem. The authors have developed mathematical models of the thermal conditions and coolant systems of hot-strip mills on the basis of a simultaneous solution of the equations of a heat balance. The mathematical model has allowed the determination of the influence of the parameters of a rolling schedule, an angle of setting guides, and also the intensity of heat interchange between the rolls and a heat-eliminating fluid on the temperature of the rolls. Engineering provisions for an increase in effectiveness of the heat removal from the rolls, that don't demand significant investment costs have been developed using the mathematical models.

10:20 AM
Distribution of Specific Force Across the Strip Width in the Roll Gap: *Eugene Nikitenko*[1]; [1]U.S. Steel Corp, Rsch. & Tech. Ctr., 4000 Tech. Ctr. Dr., Monroeville, PA 15146 USA

A new method has been developed to calculate the distribution of specific roll force along the transverse direction in the roll bite during the hot and cold rolling of strip. The method takes into account the existence of sticking and slipping zones across the strip width. A model based on the method predicts the length of the edge drop zones and can be used to improve strip crown and shape calculations.

10:45 AM Break

11:00 AM
Grinding of Strip Mill Rolls Using CBN Grinding Wheels: *Biju Varghese*[1]; Kris V. Kumar[1]; Peter Jackson[2]; [1]Diamond Innovations Inc., Engrg., 6325 Huntley Rd., Columbus, OH 43229 USA; [2]Dofasco Inc., Hot Rolling, Box 2460, Hamilton, Ontario L8N 3J5 Canada

Iron and steel mill rolls are routinely ground using grinding wheels containing conventional abrasives such as aluminum oxide. With the growing trend in the use of HSS and CPC roll materials in steel mills, it is increasingly difficult for conventional abrasive grinding wheels to resurface the rolls efficiently to achieve good profile and surface quality. This paper discusses the application of cubic Boron Nitride (cBN) grinding wheels to grind iron, HSS and CPC mill rolls. Results obtained showed the superior ability of cBN grinding wheels to produce excellent roll profile and surface quality while removing a minimum amount of roll stock. Roll stock savings greater than 50% using cBN grinding wheels have been conclusively demonstrated. Other benefits of using cBN wheels include shorter cycle time, fewer wheel changes, reduced machine maintenance and reduction in waste disposal. The use of cBN roll grinding technology has been shown to generate significant operating cost savings.

11:25 AM
Analyze for the Issue of Decreasing the Loss of Temperature in Finished Rolling of Hot Rolling Stands: *Jia Chun Xu*[1]; [1]Baosteel, Hot Rolling Mill Plant, Shanghai 200941 China

With the demands of the process in which the plate should be out of the furnace at low temperature, but should be at high temperature in rolling. So how to decrease the loss of temperature has become the focus which directly influence the quality of our products. The paper mainly analyze the reasons and reveal the main causes in finishing rolling. At the same time I put forward a few possible measures, trying to solve the problems which have disturbed us for a long time.

11:50 AM
Roll Bite Lubrication for Steel Sheet Hot Rolling: Trends and Recent Developments: *Michael Zink*[1]; James Murphy[1]; [1]Quaker Chemical Corporation, One Quaker Park, 901 Hector St., Conshohocken, PA 19428 USA

Recent technological developments in hot strip mill processing have increased the attention on roll bite lubricants (RBL). This paper and presentation present the latest advances in RBL formulation and application. Best practice and case study data will be presented including the cost-benefit analysis of using RBL versus rolling with water alone. Particular focus will be given to the interaction between RBL and newer rolling technologies such as high-speed steel rolls and strip chilling.

The Accelerated Implementation of Materials & Processes: Overviews

Sponsored by: TMS - Structural Materials Division, TMS - ASM/MSCTS-Thermodynamics & Phase Equilibria Committee, TMS - EMPMD/SMD-Chemistry & Physics of Materials Committee, TMS - MPMD-Computational Materials Science & Engineering-(Jt. ASM-MSCTS)
Program Organizers: Rollie E. Dutton, Air Force Research Laboratory, AFRL/MLLMP, WPAFB, OH 45433 USA; John E. Allison, Ford Motor Company, Materials Science and Advanced Engineering, Dearborn, MI 48124-2053 USA; John J. Schirra, Pratt & Whitney, East Hartford, CT 06108 USA; Axel van de Walle, Northwestern University, Materials Science and Engineering, Evanston, IL 60208-3108 USA

Monday AM Room: Mardi Gras Ballroom H
September 27, 2004 Location: Marriott New Orleans Hotel

Session Chair: Rollie E. Dutton, Air Force Research Laboratory, AFRL/MLLM, Wright-Patterson AFB, OH 45433-7817 USA

9:30 AM
Accelerated Insertion of Materials - Novel Disk Design and Analysis: *Peter M. Finnigan*[1]; Youdong Zhou[1]; Dominic Gao[1]; Daniel G. Backman[2]; Deb Whitis[3]; Dan Wei[2]; Steve Schrantz[3]; [1]GE Global Research Center, One Rsch. Cir., Niskayuna, NY 12309 USA; [2]GE Aircraft Engines, 1000 Western Ave., Lynn, MA 01910 USA; [3]GE Aircraft Engines, One Neumann Way, Cincinnati, OH 45215 USA

The methodology developed under DARPA's Accelerated Insertion of Materials (AIM) initiative is being implemented at GE Aircraft Engines. The AIM Designer Knowledge Base (DKB), along with the Trade Study Tool (TST), has a wide applicability throughout the design, manufacturing, and service of aerospace components. The optimization possible with the AIM DKB saves analysis time and provides the ability for synergistic design between the materials, manufacturing, and mechanical engineering disciplines. In this presentation, a variety of use cases of the AIM system will be described, specifically the analysis of a dual heat-treated disk and inverse modeling to achieve heat transfer coefficients (HTCs) during the heat treat process.

9:55 AM
Linking Processing and Performance of Engineering Materials Through Microstructure Explicit Modelling: *Malcolm McLean*[1]; Peter D. Lee[1]; Sammy Tin[2]; [1]Imperial College London, Dept. of Matls., Exhibition Rd., London SW7 2AZ UK; [2]University of Cambridge, Rolls Royce UTC, Pembroke St., Cambridge CB2 3QZ UK

Quantitative measures of material microstructure are an output of multiscale models of material processing. They are also the starting points for advanced models of material behaviour. This paper describe the approach being taken to integrate the process and behaviour models, with appropriate experimental validation at each stage, to simulate the likely behaviour of components in service resulting from variations in process conditions. The approach will be illustrated by contributions to turbine disc technology drawn from two inter-institutional collaborative programmes: 1) Models of individual stages of turbine disc manufacture (ingot production, heat treatment, cogging, forging) have been linked to track the evolution of grain structure and the location of inclusions. This work formed part of the EPSRC IMMAD collaboration with Universities of Cambridge and Birmingham, Special Metals and Rolls Royce. 2) A microstructure-explicit model of creep of turbine disc alloys has been developed as part of the DARPA AIM programme in conjunction with GE Aircraft Engines, Pratt & Whitney and their consortia of university partners. Progress to incorporating the spatial and temporal variations of microstructure in engineering components into the constitutive descriptions of mechanical behaviour will be discussed.

10:20 AM
Direct Simulation of Fatigue Properties Using Microstructural Models: *Robert G. Tryon*[1]; Animesh Dey[1]; Ganapathi Krishnan[1]; Yaowu Zhao[1]; [1]VEXTEC, 750 Old Hickory Blvd., Bldg. 2, Ste. 270, Brentwood, TN 37027 USA

Computational material response algorithms have been developed to simulate the fatigue behavior of metallic components based on the material microstructure. The purpose of the algorithms is to assess the microstructural effects such that changes in microstructure can be quantitatively related to the fatigue response. The fatigue process is divided into three phases. The first phase is the crack nucleation phase in which damage accumulates to form a crack in an initially uncracked structure. The second phase is the small crack growth phase in which the crack size is on the order of the microstructure. The third phase is the long crack growth phase in which the crack size is large compared to the microstructure. Monte Carlo simulation software is developed that uses dislocation theory based critical damage models. Probabilistic methods are used to predict the statistical variation in the fatigue response due to the random nature of the physical microstructure.

10:45 AM Break

11:00 AM
The AIM Method Applied to the Qualification of UHS Stainless Landing Gear Steel: *Charles J. Kuehmann*[1]; [1]QuesTek Innovations LLC, 1820 Ridge Ave., Evanston, IL 60015 USA

The Accelerated Insertion of Materials methods, developed under DARPA sponsorship, are being applied to the qualification of an ultra-high strength stainless steel for landing gear applications. The alloy, Ferrium S53, was designed using computational materials design methods with mechanical property targets equivalent to 300M steel and corrosion resistance similar to 15-5PH stainless. The alloy has demonstrated primary property and processing goals within a Strategic Environmental Research and Development Program and is now in qualification in an Environmental Strategic Technology Certification Program within the DoD. The AIM strategy applied to Ferrium S53 will predict MIL-HNDBK-5 A-allowables property values for ultimate tensile strength and fatigue strength with data from only three production heats of material. The approach will integrate computational modeling and AIM methods to achieve the accelerated insertion of Ferrium S53 into USAF applications within three years. A review of the approach and progress to date will be presented.

11:25 AM Invited
Computational Crystal Structure Prediction: *Dane Morgan*[1]; Gerbrand Ceder[1]; Stefano Curtarolo[2]; [1]Massachusetts Institute of Technology, Matls. Sci., 77 Mass. Ave., 13-4061, Cambridge, MA 02139 USA; [2]Duke University, Mechl. Engrg. & Matls. Sci., 144 Hudson Hall, Box 90300, Durham, NC 27708 USA

Atomistic based computational materials design holds great promise for accelerating the pace of materials development. Although atomistic calculations can determine many important properties, an approximate initial structure must be provided. Unfortunately, at this point there is no general tool for reliably predicting crystal structure of new alloys, which will become increasingly limiting as atomistic methods explore more new materials. Total energy ab initio approaches can be used to directly compare energies of different candidate structures, but developing a manageable list of candidate structures for comparison is still very challenging. A novel data mining framework will be introduced for mining existing data, both computational and experimental, to predict likely structures for new alloys. Initial tests of this combined data mining and computational approach will be shown to dramatically decrease the time needed to identify stable crystal structures.

11:50 AM
Structural Materials for Terrestrial and Space Nuclear Applications: *S. J. Zinkle*[1]; [1]Oak Ridge National Laboratory, 1 Bethel Valley Rd., PO Box 2008, Oak Ridge, TN 37831-6138 USA

High performance materials are critical for success in both terrestrial and space nuclear applications. Nuclear power currently accounts for about 20% of the US electricity and ~24% of the worldwide electricity. Looking to the future, advanced fission ("Generation IV") and fusion reactor systems are proposed to meet the growing worldwide energy demand and to reduce reliance on fossil fuel energy sources that produce greenhouse gases. In response to increasing scientific payload electricity demands for proposed space missions, NASA recently initiated an advanced technology program that will enable several nuclear space reactor missions including orbiter exploration of the moons of Jupiter. This paper will compare and contrast the performance requirements and summarize candidate structural materials in existing fission reactors, proposed fusion and Generation IV fission reactors, and proposed space reactors. The structural materials requirements for existing fission reactors include good strength for long times (>40 years) at moderate temperatures, adequate resistance to mechanical property degradation (fracture toughness, etc.) by irradiation, and chemical compatibility with coolants (water, Na). Thermal creep and neutron radiation resistance will be of very high importance for structural materials in proposed Generation IV reactors, due to the significantly higher operating temperatures and neutron exposure levels compared to existing fission reactors. Structural materials in proposed fusion reactors will experience similar high temperature and neutron dose demands as Generation IV reactors, but the higher neutron energies associated with fusion will cause additional radiation damage challenges. In addition, use of alloying elements that do not lead to long-lived radioactivity is considered essential for the development of fusion. Due to the requirement to minimize launch mass for space power and propulsion systems (typical launch costs are 10 to 40 k$/pound), high thermal efficiency is essential in space reactor systems. This leads to high operating temperatures for the structural materials, with most attention focused on refractory alloys. Thermal creep, neutron radiation resistance, and chemical compatibility with the coolant (Na, Li) are the main concerns for space reactor structural materials.

Third International Symposium on Railroad Tank Cars: Session I

Sponsored by: AIST, AIST - Division VI
Program Organizers: Murali Manohar, ISG; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Monday AM — Room: Mardi Gras Ballroom B
September 27, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Murali Manohar, International Steel Group Research, Bethlehem, PA 18015-4731 USA; Geoff Dahlman, Burlington Northern Santa Fe Railway, Techl. R&D, Topeka, KS 66612 USA

9:30 AM
The Physical Metallurgy of Normalized Plate Steels: *Richard L. Bodnar*[1]; Frederick B. Fletcher[1]; Murali Manohar[1]; [1]International Steel Group, Rsch., 112 Rsch. Dr., Bethlehem, PA 18015-4731 USA

Normalizing of steel plates is primarily used to enhance toughness, refine ferrite grain size, reduce the variability in mechanical properties, and produce a uniform microstructure throughout the product thickness. Although the normalizing process has been used in the production of steel plates for many years, our understanding of the physical metallurgy of such steels continues to evolve. This paper reviews the physical metallurgy of normalized ferrite-pearlite and ferrite-pearlite-bainite steel plates. The effects of carbon and other elements in steel, prior structure, normalizing temperature, cooling rate, and stress relieving/tempering will be discussed. Recently developed data on the effects of niobium and titanium will also be presented.

10:30 AM
Impact Resistance of Steel from Derailed Tank Cars in Minot, ND: *Frank P. Zakar*[1]; [1]National Transportation Safety Board, Matls. Lab., 490 L'Enfant Plaza E., Washington, DC 20594 USA

On a freezing morning in January 2002, a freight train derailed in Minot, North Dakota, causing five tank cars that carried anhydrous ammonia to catastrophically rupture. The event led to immediate release of over 142,000-gallons of anhydrous ammonia, posing a great hazard to the local community. Charpy V-notch impact testing of samples removed from the shell portions of several catastrophically fractured tank cars showed that the impact resistance of the steel for each tank car varied greatly. The NTSB metallurgical investigation also determined that brittle fractures and low impact resistance of the steel contributed to the catastrophic fracture of the tank cars. The paper will discuss the results of Charpy V-notch impact testing of selected tank cars from the catastrophically fractured tank cars, and will share thoughts on which direction the tank car community should proceed to improve the construction of future tank cars.

11:00 AM
Effect of Nb on Weld Heat Affected Zone Toughness of Normalized C-Mn Tank Car Steel: *Chirag G. Shah*[1]; Philip Nash[2]; [1]Bodycote Materials Testing Inc., 7530 Frontage Rd., Skokie, IL 60077 USA; [2]Illinois Institute of Technology, Thermal Procg. Tech. Ctr., 10 W. 32nd St., Chicago, IL 60616 USA

The influence of Nb on the toughness of weld heat-affected zone in normalized carbon-manganese-vanadium steel in the post weld heat-treated and as welded conditions was studied. Four special laboratory heats were made with composition similar to tank car steel AAR TC 128B and allowing only the Nb content to vary. Gleeble simulation was performed to reproduce thermal cycles typically encountered in weld HAZ's during tank car fabrication. Also, submerged arc welds were made on the plates using parameters typically used in tank car fabrication to prepare real weldment specimens. Full size Charpy specimens from the heat affected zone of the simulated and real weldment specimens were machined and tested per ASTM E-23. Good correlation was observed between the real weldment and simulated samples test results. Acceptable PWHT heat affected zone toughness at -30°F was obtained only with the lowest (< 0.005%) Nb containing steel simulated using lower heat input of 76.2 kJ/inch. The adverse influence of Nb, especially in the post weld heat-treated condition was demonstrated. Some possible mechanisms by which Nb could reduce heat affected zone toughness are discussed and suggested future work is outlined.

3-Dimensional Materials Science: Serial Sectioning II

Sponsored by: TMS - Structural Materials Division
Program Organizers: Marc J. De Graef, Carnegie Mellon University, Department Material Science & Engineering, Pittsburgh, PA 15213-3890 USA; Jeff P. Simmons, Air Force Research Laboratory, Materials & Manufacturing Directorate, Dayton, OH 45433 USA; George Spanos, Naval Research Laboratory, Physical Metallurgy Branch, Washington, DC 20375-5000 USA; Jonathan E. Spowart, UES Inc., Dayton, OH 45432 USA

Monday PM Room: Mardi Gras Ballroom F/G
September 27, 2004 Location: Marriott New Orleans Hotel

Session Chairs: Michael Uchic, Air Force Research Laboratory, AFRL/MLLMD, Wright Patterson AFB, OH 45433-7817 USA; Alexis C. Lewis, Naval Research Laboratory, Code 6352, Washington, DC 20375 USA

2:00 PM
3D Reconstruction of Titanium Boride and Alpha Precipitates in Titanium Alloy Based Metal-Matrix Composites: *Davion Hill*[1]; Robert Williams[1]; Peter Collins[1]; Rajarshi Banerjee[1]; Hamish Fraser[1]; [1]Ohio State University, Matls. Sci. & Engrg., 477 Watts Hall, 2041 College Rd., Columbus, OH 43210 USA

Metal-matrix composites usually consist of hard dispersoids, such as transition-metal carbides or borides, dispersed in a tougher alloy matrix. An example of such a composite is the titanium boride (TiB) in titanium alloy matrix system. During the processing of these metal-matrix composites the TiB precipitates form during the solidification of the alloy which is followed by the solid-state precipitation of alpha in the beta titanium + TiB matrix as the alloy cools below the alpha-beta transus temperature. During the solid-state precipitation of alpha in a matrix of beta titanium, the presence of TiB precipitates act as additional nucleation sites for the alpha phase. Furthermore, the alpha nucleated on the TiB precipitates exhibit an equiaxed or globular morphology in contrast to the alpha precipitated on other nucleation sites such as grain boundaries, which exhibit a more lath-like morphology. Details of the precipitation process and the morphologies of the various phases involved, TiB and alpha Ti, have been investigated using three-dimensional tomography. A Dual-beam FIB has been used for serial-sectioning of the microstructure and imaging using a custom-built backscatter SEM detector installed in the FIB. Subsequently, these serial sections have been used for reconstructing the microstructure in three dimensions within the framework of the IMOD software. These results and their implications on the evolution of microstructure in the TiB composites will be discussed in this presentation.

2:20 PM
Three-Dimensional Analysis of a Superaustenitic Stainless Steel: *Alexis C. Lewis*[1]; Andrew Geltmacher[2]; George Spanos[2]; [1]National Research Council, Washington, DC 20001 USA; [2]Naval Research Laboratory, Code 6300, Washington, DC 20375-5000 USA

The US Navy is currently interested in non-magnetic steels with high strength, toughness, and corrosion resistance. As part of a multidisciplinary "Materials By Design" program at the Naval Research Laboratory, microstructural evolution in AL-6XN, a commercial superaustenitic stainless steel, has been investigated. The 3-D morphology, distribution, and crystallographic orientation of the matrix austenite grains, as well as boundary types and inclinations, have been characterized using serial sectioning and 3-D reconstruction in conjunction with Electron Backscatter Diffraction (EBSD). In addition, 3-D morphology and crystallography of a second phase (sigma) precipitate was investigated. These 3D reconstructions have been supplemented by Focussed Ion Beam (FIB) "deep etching" and cutting of orthogonal surfaces. The reconstructions of the structure, interconnectivity, and orientation of the matrix austenite grains that will be shown here are also used as input into a 3-D image-based materials response model of stress and strain evolution. (The details of this model will be presented at another talk in this symposium). In addition to demonstrating the true 3-D microstructure of this steel, this presentation will briefly review some details of the 3-D techniques employed.

2:40 PM Invited
3D Visualization of Scientific Datasets with VTK: *Will Schroeder*[1]; [1]Kitware, Inc., 28 Corporate Dr., Ste. 204, Clifton Park, NY 12065 USA

The Visualization Toolkit is a freely available, open-source system supporting image processing, 3D graphics, data visualization and volume rendering. Implemented in C++, VTK is portable across Linux, Windows, and Mac platforms and provides bindings to the Tcl, Java, and Python programming languages. The toolkit is used around the world by research, educational, and commercial organizations. The VTK community is large consisting of approximately 2500 subscribers on its mailing lists, documentation in the form of professional books and on-line manuals, and commercial support from Kitware, Inc. VTK is under active development and is funded by such prestigious organizations as the US National Labs Los Alamos, Sandia and Livermore and the Army Research Labs. This talk will provide an overview of VTK and its use in applications including supercomputing, medical visualization, and numerical simulation. The talk will also provide an overview of several turnkey applications built on top of VTK including the large data visualization tool ParaView and the volume rendering system VolView.

3:25 PM Break

3:55 PM
Reconstructed Alpha Lath Morphology of Titanium Alloys from Serial Sectioning in a Dual Beam FIB: *Robert E.A. Williams*[1]; Rajarshi Banerjee[1]; Michael Uchic[2]; Dennis M. Dimiduk[2]; Hamish L. Fraser[1]; [1]Ohio State University, 2041 College Rd., Columbus, OH 43210 USA; [2]Air Force Reasearch Laboratory, Matls. & Mfg. Direct., AFRL/MLLMD, Bldg. 655, 2230 Tenth St., Wright Patterson AFB, OH 45434-7817 USA

The development of a set of robust computational tools that permit microstructurally-based prediction of mechanical properties for commercially important Titanium alloys is important to the accelerated maturation of materials. In order to facilitate the accurate development of a predictive model, 3-D reconstructions of complex microstructures found in Titanium alloys is vital. Commercial software, Slice and View™, has been used in a dual beam FIB to serial section through approximately 8 microns of material in a single run. Due to the amount of beam shift in the FIB, however, it is nearly impossible to increase the depth of sectioning with successive runs while maintaining the desired field of view using Slice and View™. A custom script has been developed that allows for stage movement and realignment of the viewing area through the use of fiducial markers. Currently, the dual beam FIB has been used to section through 50 microns of material in a single run with use of the modified script. Alpha laths have been reconstructed in near alpha, alpha plus beta, and near beta Titanium alloys. This talk will address the varying morphology of alpha laths and present 3-D reconstructions from the different Titanium alloys. Sample preparation technique, both external and in-situ will be discussed as well as preliminary thoughts for quantification of the alpha lath.

4:15 PM
Three-Dimensional Analysis of Coarse Martensite in Low Carbon Steels: *George Spanos*[1]; Alexis C. Lewis[1]; Archana Gupta[2]; [1]Naval Research Laboratory, Code 6324, 4555 Overlook Ave., Washington, DC 20375-5000 USA; [2]GeoCenters, Inc. (stationed at the Naval Research Laboratory), Fort Washington, MD 20749 USA

Previous studies have reported on a very coarse autotempered plate martensite which forms during continuous cooling at fast rates in certain low carbon steels (e.g., HSLA-100); these studies indicated that the morphology of this martensite may resemble a plate shape. In the present research, serial sectioning and 3-D reconstruction and scientific visualization techniques were employed to elucidate the true 3-D morphology and interconnectivity of these coarse martensite crystals. This work is the follow on study of preliminary results and methodologies presented previously. Current results show that these large martensite crystals (?20 microns in length) often exhibit a 3-D morphology which differs considerably from the classic views of either fine lath (dislocated) martensite or coarse plate (twinned) martensite. The coarse martensite observed here forms with one flat edge and one sharp/knife edge; both of these edges run the length of the long axis. Further details of the growth "tips" of these martensite crystals, and their different morphological details and interconnectivities in 3D will be presented. The 3-D results will also be briefly correlated to Transmission Electron Microscopy (TEM) observations, which indicate (among other things) that these crystals contain no internally twinned structure and no obvious midribs. The 3-D findings will also be correlated to Electron Backscatter Diffraction (EBSD) analyses, which will be presented in detail in another symposium at this conference. Finally, details of the formation mechanism of this microconstituent will be discussed in light of the current observations.

4:35 PM
3D Analysis of Creep Voids in Hydrogen Reformer Tubes: *Azmi Abdul Wahab*[1]; Milo V. Kral[1]; [1]University of Canterbury, Mechl. Engrg., PO Box 4800, Christchurch 00000 New Zealand

Hydrogen reformer tubes typically fail by formation and coalescence of creep voids during service. Crystallographic parameters, local geometry, and stress influence the exact locations of these voids. In the present work, ex-service hydrogen reformer tubes composed of Fe-35% Ni-25% Cr-1.5% Nb-0.50% C-2.0% Si-1.5% Mn (approximate wt%) were examined via a serial sectioning technique to obtain a volume data set of void locations for three-dimensional reconstruction and analysis. Crystallographic orientation maps of the sectioned area were periodically collected using electron backscatter diffraction (EBSD) pattern analysis. Correlation between local stress state, crystallography and microstructure will be presented.

Computational Microstructure Evolution in Steel: Stress, Strain and Deformed Microstructures

Sponsored by: TMS - Structural Materials Division, TMS - EMPMD/SMD-Chemistry & Physics of Materials Committee, TMS - MPMD-Computational Materials Science & Engineering-(Jt. ASM-MSCTS)
Program Organizers: Koenraad G.F. Janssens, Sandia National Laboratories, Materials and Process Modeling, Albuquerque, NM 87185-1411 USA; Mark T. Lusk, Colorado School of Mines, Mechanical Engineering Program, Division of Engineering, Golden, CO 80401 USA

Monday PM Room: La Galerie 4
September 27, 2004 Location: Marriott New Orleans Hotel

Session Chair: Koenraad G.F. Janssens, Sandia National Laboratories, Albuquerque, NM 87185 USA

2:00 PM Invited
On Dislocation Dynamics: *Hussein M. Zbib*[1]; [1]Washington State University, Sch. of Mechl. & Matls. Engrg., Pullman, WA 99164-2920 USA

Abstract not available.

2:40 PM
Three-Dimensional Instability of a Retracting Film Edge: *Wanxi Kan*[1]; Harris Wong[1]; [1]Louisiana State University, Mechl. Engrg., Baton Rouge, LA 70803 USA

When bonding two stainless steel surfaces, uniform interfacial layers such as Ti sometimes are deposited on the surfaces to assist bonding. The thickness of the interfacial layer is usually in the range of nano-meters. Under certain conditions, a semi-infinite uniform film on a substrate can evolve to reduce the surface energy and agglomerate below the melting temperature of the film. This work studies the three-dimensional instability of a solid film step, assuming that the film evolves by capillarity-driven surface diffusion. It is found that growth rate of the perturbation depends on the velocity of the moving boundary and the wavelength of the perturbation. The faster the film boundary moves, the more unstable the film is. When the wavelength of the perturbation exceeds a critic value, the film is always unstable. This explains the formation of fingers observed in the breakup of gold films.

3:00 PM
Grain Boundary Grooving by Surface Diffusion with Strong and Asymmetric Surface Energy Anisotropy: *Donghong Min*[1]; *Harris Wong*[1]; [1]Louisiana State University, Mechl. Engrg. Dept., Baton Rouge, LA 70803 USA

Surface energy anisotropy can affect magnetic anisotropy of low silicon steels. We study surface energy anisotropy effects on grain-boundary grooves. A vertical grain boundary of a bicrystal forms a groove at a free surface to reduce the combined surface energy. The grain-boundary grooving is driven by surface diffusion with strong and asymmetric surface energy anisotropy. A recently developed spike function facet model is used to prescribe the anisotropy. The partial differential equation governing surface diffusion is reduced to a set of ordinary differential equations by a self-similar transformation and solved numerically by a shooting method. It is found that the shape of the free surface is a function of the contact angle α(surface orientation parameter) and the facet angle β (facet orientation parameter). Depending on α and β, the groove profile can be smooth or faceted on one side or both sides. Computed profiles agree with one $SrTiO_3$ bicrystal sample experiment in which $\alpha = \beta = 0.4°$.

3:20 PM Break

3:40 PM Invited
Prediction of Plastic Anisotropy and Deformation Textures of Steel Using Mesoscopic Models: *Paul R. Van Houtte*[1]; Marc Seefeldt[1]; Albert Van Bael[1]; Laurent Delannay[2]; [1]Katholieke Universiteit Leuven, MTM, Kasteelpark Arenberg 44, Leuven BE-3001 Belgium; [2]Université Catholique de Louvain, CESAME-MEMA, Bâtiment Euler, Av. Georges Lemaître,4, Louvain-la-Neuve BE-1348 Belgium

Various statistical models for the plastic deformation of polycrystals are reviewed. They model the behaviour of randomly chosen individual grains, after which a homogenisation is performed. Their purpose is to predict the evolution of the crystallographic texture and to generate the anisotropic stress-strain relationship. Some of these are classical statistical models such as the Taylor model, the relaxed constraints model and the self-consistent model. The more recent 'interaction' models focus on the interaction between adjacent grains: the GIA, LAMEL and ALAMEL models. The most sophisticated interaction model is the crystal plasticity finite element model (CPFEM), but it requires a calculation effort which is orders of magnitude larger than the three other interaction models. The differences between all these models will be discussed from the viewpoints of homogenization; microstructure and dislocation pattern modelling. Validations of rolling texture predictions for IF steel and aluminium alloys will be reported.

4:20 PM
Phase Field Modeling of Stress-Strain Evolution During Austenite to Ferrite Transformation in Low C Steels: *Markus Apel*[1]; Ingo Steinbach[1]; [1]Access e. V., Intzestr. 5, Aachen 52072 Germany

Solid state transformations are strongly influenced by elastic stresses if they are associated with volume changes. The elastic energy usually slows down the rate of transformation by creating an additional energy barrier against transformation. We present an extended multiphase field model that calculates the effect of elastic stress on phase transitions in polycrystalline multiphase systems. The model avoids homogeneous approximation, by that allowing to study the effect of different elastic properties or orientations of individual grains. We will discuss the effect of elastic stress and strain on austenite to ferrite transformation kinetics as well as morphology. The importance of elastic energy contribution to nucleation and initial growth kinetics of ferritic grains in the austenitic matrix will be investigated. The cubic symmetry of the elastic properties leads to stress induced anisotropy in the growth kinetics. The relevance of this anisotropy for the morphology of Widmannstaetten ferrite will be discussed.

Continuous Casting Fundamentals: Initial Solidification and Interfacial Phenomena

Sponsored by: AIST, TMS, AIST - Division VI, AIST - Division VII, TMS - MPMD-Solidification Committee, TMS - MPMD/EPD-Process Modeling Analysis & Control Committee
Program Organizers: Brian G. Thomas, University of Illinois, Department of Mechanical and Industrial Engineering, Urbana, IL 61801 USA; Michael Byrne, International Steel Group, Homer Research Labs, Bethlehem, PA 18016 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Monday PM Room: Grand Ballroom M
September 27, 2004 Location: Marriott New Orleans Hotel

Session Chairs: Brian Thomas, University of Illinois, Dept. of Mechl. & Indust. Engrg., Urbana, IL 61801 USA; Michael Byrne, International Steel Group, Homer Rsch. Labs, Bethlehem, PA 18016 USA

2:00 PM Opening Remarks

2:05 PM Keynote
Initial Solidification of Steel in a Continuous Casting Mold: *Alan W. Cramb*[1]; [1]Carnegie Melon University, Dept. of Matls. Sci. & Engrg., 5000 Forbes Ave., Pittsburgh, PA 15213 USA

How does solidification start and progress in a continuous casting mold? This is a key question in the development of both surface quality and cast structure and is not completely understood at this time. In this presentation our current understanding of the formation of solid steel in a continuous casting mold will be discussed. Both micro and macro solidification phenomena will be outlined with reference to the formation of the cast surface. Meniscus phenomena including oscillation marks and subsurface defects will be elucidated.

2:40 PM
Analysis of Hook Formation Mechanism in Ultra Low Carbon Steel Using CON1D Heat Flow - Solidification Model: *Ho-Jung Shin*[1]; Go-Gi Lee[1]; Seon-Hyo Kim[1]; *Brian G. Thomas*[2]; [1]Pohang University of Science and Technology, Dept. of Matls. Sci. & Engrg., San 31, Hyoja-dong, Nam-gu, Pohang, Kyungbuk 790-784 Korea; [2]University of Illinois, Dept. of Mechl. & Indust. Engrg., 356 Mechl. Engrg. Bldg., MC-244, 1206 W. Green St., Urbana, IL 61801 USA

Subsurface hook formation at the meniscus during the continuous casting of steel slabs is an important cause of surface defects, owing to their easy entrapment of mold flux and inclusion-laden gas bubbles. This work investigates the fundamentals of meniscus solidification and how hooks form by a combination of advanced computational models and plant measurements. The model predicts shell growth at the meniscus, heat transfer across the interfacial flux layers, and temperature in the mold. These computational results compare well with experimental measurements of hook thickness conducted on cast slabs under different casting conditions.

3:05 PM
The Effect of Phase Diagram Information on Modeling Peritectic Reaction Rates: *Neill John McDonald*[1]; Sridhar Seetharaman[1]; [1]Carnegie Mellon University, Matls. Sci. & Engrg. Dept., 5000 Forbes Ave., Pittsburgh, PA 15213 USA

The peritectic transition is an important phenomenon for many ferrous alloys, especially during the continuous casting process. Many defects have been attributed to this high-temperature phase change, including break-outs, longitudinal cracking, and transverse facial cracking. Observations have been made and reported of the shape and rate of advancement of the delta-ferrite/austenite/liquid junction for Fe-C, Fe-Ni, Fe-Co, and Fe-Cr-Ni alloys using the high-temperature Confocal Scanning Laser Microscope at Carnegie Mellon University. All diffusion control models used to describe this peritectic reaction rate have shown large dependencies on phase diagram information - namely, the liquidus, solidus, and solvus curves as well as the size of the two-phase ferrite/austenite and austenite/liquid fields. An investigation of available phase diagrams has been made along with a comparison against thermodynamic principles. The effect of diffusivity and phase diagram data on the predicted rate of peritectic reaction was then examined and a contrast against observed rates completed.

3:30 PM Break

3:40 PM
Effects of Oxides on the Undercooling of Pure Iron: *Martin Emiliano Valdez*[1]; Hiroyuki Shibata[2]; Sridhar Seetharaman[1]; Alan W. Cramb[1]; [1]Carnegie Mellon University, Dept. Matls. Sci. & Engrg., 5000 Forbes Ave., Wean Hall 2307, Pittsburgh, PA 15213 USA; [2]Tohoku University, Inst. of Multidisciplinary Rsch. for Advd. Matls., 2-1-1 Katahira Aobaku, Sendai 980-8577 Japan

The properties of continuous casting products strongly depend on the solidification structure, namely the size of columnar and equiaxed zones and the grain size distribution. The nucleation of an equiaxed grain is mainly determined by the availability of nucleation sites and the presence of an undercooled liquid either at the surface or center of a casting. The use of non-metallic inclusions as effective nucleation sites has received significant attention in recent years. This paper will discuss the potential for significantly undercooling pure iron on different substrates by varying atmospheric conditions.

4:05 PM
The Effect of Surface Oxide Films on Heat Transfer Behavior in Strip Casting Process: *Paolo Nolli*[1]; Alan W. Cramb[1]; Dong-Kyun Choo[2]; [1]Carnegie Mellon University, Matls. Sci. & Engrg., 5000 Forbes Ave., Wean Hall, Pittsburgh, PA 15213 USA; [2]Research Institute of Industrial Science and Technology, Mgmt. Project Team, #32, Hyoja Dong, Pohang 790-330 S. Korea

In the last few years many companies have announced the final stage of the development in the strip casting of some steel grades. In strip casting, the initial solidification behavior of the solidified shell is crucially important to achieve good quality of steel strip. Thus, much attention has been paid to the heat transfer behavior in the initial stage of the solidification process. Among many factors influencing heat transfer, oxide films, either formed during casting or deposited before it on the surface of the rolls, could have a significant effect. The heat transfer behavior of different kinds of steels and the effect of different deposited oxides have been evaluated by using an apparatus designed for millisecond resolution in heat transfer measurements, and by analyzing the formation mechanism of oxide films on the mold surface. The microstructure of the solidified shell resulting from the experiments has been analyzed and has shown the corresponding dependency between microstructure evolution and heat transfer behavior.

4:30 PM
Mold Slag Property Measurements to Characterize CC Mold - Shell Gap Phenomena: *Ya Meng*[1]; Brian G. Thomas[1]; Andreas A. Polycarpou[1]; Hani Henein[2]; Arvind Prasad[2]; [1]University of Illinois, Mechl. & Indust. Engrg., 1206 W. Green St., Urbana, IL 61801 USA; [2]University of Alberta, Chem. & Matls. Engrg., 536 Min. Chem. Engrg. Bldg., Edmonton, Alberta T6G 2G6 Canada

Multi-faceted experiments were conducted to measure the properties of several mold slags, needed for fundamental characterization of heat transfer and friction in the interfacial gap between the shell and mold during the continuous casting of steel. A novel apparatus was used to measure the friction coefficient between solidified mold flux and copper at elevated temperature. The measured softening temperature is interpreted to extrapolate the slag viscosity-temperature curves far into the low temperature - high viscosity region. Continuous-cooling transformation curves were extracted from XRD analysis of DSC test samples and thermocouple dip tests. Time-temperature transformation curves were obtained from similar analysis of melted mold powder samples that were atomized into droplets, quenched to form glass, and then partially devitrified by reheating to different temperatures for different times and quenched. Polarized light microscopy, SEM, and EDX analysis revealed distinct crystalline and glassy layers, but no severe macro-segregation in a tail-out slag film taken from an operating caster. The results from these new measurements have important implications for the prediction of interfacial gap phenomena, including mold heat transfer, friction, slag layer fracture, and steel surface quality.

4:55 PM
Study of Free-Fluoride Mold Powder Based on Titanium-Bearing Blast Furnace Slag: *Guang Hua Wen*[1]; Ping Tang[1]; Miao Sheng Tian[1]; Yong Qing Liu[1]; [1]Chongqing University, College of Matls. Sci. & Engrg., Shazhengjie 174#, Chongqing 400044 China

Fluorine is mostly come from mold powder in the continuous casting process. The research on the free-fluoride mold powder has an important role in environmental protection. The titanium-bearing blast furnace slag of Pangzhihua Iron and Steel Company in China is used as a base material of free-fluoride mold powder to control the mold heat transfer in this paper. The effects of fusion agent type and adding quantity, basicity, content of TiO2 in CaO-SiO2-TiO2 slag on viscosity, melting and crystallization temperature of free-fluoride mold powder are studied. The trial result cast peritectic steel indicates that surface quality of the slab is good and the free-fluoride powder can effectively control mold heat transfer for perovskite in the flux instead of cuspidine in fluoride-bearing flux.

General Abstracts: Mechanical Behavior & Characterization

Sponsored by: AIST, TMS
Program Organizers: Dennis M. Dimiduk, Air Force Research Laboratory, Materials & Manufacturing Directorate, WPAFB, OH 45433 USA; E. Buddy Damm, The Timken Company, Canton, OH 44706-0930 USA; James C. Foley, Los Alamos National Laboratory, Los Alamos, NM 87545 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Monday PM — Room: Mardi Gras Ballroom A
September 27, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Peter M. Sarosi, Ohio State University, Dept. of Matls. Sci. & Engrg., Columbus, OH 43210 USA; David A. Johnson, Air Force Research Laboratory, Matls. & Mfg. Direct., Wright-Patterson AFB, OH 45433-7817 USA

2:00 PM
Mechanical Testing and Structure Characterization of TBC Bond Coats and Thermally Grown Oxides: *Cristian Cionea*[1]; Kevin J. Hemker[1]; [1]Johns Hopkins University, Mechl. Engrg. Dept., 3400 N. Charles St., 223 Latrobe, Baltimore, MD 21218 USA

Bond Coat and thermally grown oxide (TGO) mechanical properties are considered to be important factors that contribute to the failure mechanism of thermal barrier coating systems. In order to address this subject, several bond coats have been developed by modifying the alloying elements in the superalloy substrate. It is believed that those elements diffuse into the bond coat and influence its mechanical behavior at high temperatures (700-11500 C). Yield strength and Young's modulus were measured from microsample tensile tests, and stress relaxations tests were performed to obtain the creep behavior of the bond coats. The results will be discussed in light of the chemical composition of the various bond coats. A technique for high temperature testing of the 5 micron TGO is being developed and will also be presented.

2:20 PM
Location Specific In-Situ TEM Straining Specimens Using FIB: *R. D. Field*[1]; P. A. Papin[1]; [1]Los Alamos National Laboratory, MST-6, MS G770, Los Alamos, NM 87545 USA

A method has been devised and demonstrated for producing in-situ straining specimens for the Transmission Electron Microscope (TEM) from specific locations in a sample using a Dual Beam Focused Ion Beam (FIB) instrument. The specimen is removed from a polished surface in the FIB using normal methods and then attached to a pre-fabricated substrate in the form of a modified TEM tensile specimen. In this manner, specific features of the microstructure of a polished optical mount can be selected for in-situ tensile straining. With the use of Electron Backscattered Electron Diffraction (EBSD), this technique could be extended to select specific orientations of the specimen as well. Details of the technique will be presented, along with experimental results.

2:40 PM

Microsample Characterization of Coatings for GRCop-84 for High Temperature High Heat Flux Application: *Piyush Jain*[1]; Kevin J. Hemker[1]; Sai V. Raj[2]; [1]Johns Hopkins University, Mechl. Engrg., 3400 N. Charles St., 22 Latrobe Hall, Baltimore, MD 21218 USA; [2]Nasa Glenn Research Center, 21000 Brookpark Rd., Cleveland, OH 44135 USA

NASA's Glenn Research Center has developed GRCop-84 (Cu-8at.%Cr-4%Nb), a high conductivity, high strength copper alloy for use as liners in rocket engine combustion chambers, nozzle ramps and other actively-cooled components subject to high heat fluxes. Two metallic coatings, NiCrAlY and Cu-26%Cr, are being considered for preventing blanching, reducing 'dog-house' failures and providing better environmental resistance to the GRCop-84 liners. This presentation will outline a study of coating-substrate interactions that occur as a result of thermal cycling and coating specific properties at different temperatures. A furnace has been built to thermally cycle the samples under argon. The microsample testing approach is being used to measure the coating-substrate interfacial strength. Cu-26Cr/GRCop-84 samples did not show any obvious interdiffusion after 300 thermal cycles. Interfacial strength tests of these samples were affected by porosity present in the samples. A complete set of observations and results for Cu-26Cr and NiCrAlY coatings will be presented.

3:00 PM

High Temperature Creep Behavior of Binary Ti-6Al Alloys with Trace Amounts of Ni: *Jun ho Moon*[1]; S. Karthikeyan[1]; G. B. Viswanathan[1]; R. W. Hayes[2]; S. P. Fox[3]; M. J. Mills[1]; [1]Ohio State University, Dept. of Matls. Sci. & Engrg., 2041 College Rd., 477 Watts Hall, Columbus, OH 43210 USA; [2]Metals Technology Inc., 19801 Nordhoff, Northridge, CA 91324 USA; [3]Timet Inc., America Techl. Lab., W. Lake Mead & Atlantic Ave., Henderson, NV 89015 USA

The high temperature creep behavior of two binary, equiaxed Ti-6Al alloys with varying trace amounts of Ni (<3ppm and 3ppm) was studied. Creep tests were performed in uniaxial compression over the temperature range 510 to 593°C at applied stress levels ranging from 150 to 300MPa. Stress and temperature jump tests were performed to obtain the stress exponents and the creep activation energy. The results show that increased amounts of Ni increased the minimum creep rates at all stress levels. Stress exponent values of ~5.0 were obtained for both samples. Detailed TEM analysis of the deformation structure was performed on samples crept monotonically at 200~300MPa up to 0.2~4.5% plastic strain. The results are explained with reference to the recently reported trends associated with lattice self-diffusion in alpha-titanium in the presence of fast diffusing impurities. Analysis of the dislocation structures along with the possible creep mechanism is presented.

3:20 PM

Recovery of Strain Hardening in Creep Deformed Ti-6 wt% Al Alloys: *Charles M. Brandes*[1]; Michael J. Mills[1]; [1]Ohio State University, Dept. of Matls. Sci. & Engrg., 477 Watts Hall, 2041 College Rd., Columbus, OH 43210 USA

A short time ago, Ti-Al alloys were found to undergo marked recovery of strain hardening following creep deformation at low stresses and temperatures. This phenomenon was observed in specimens that had been crept in compression to a given level of plastic strain, unloaded, aged at ambient temperature for a period of days, and reloaded at the initial stress level. Remarkably, the strain rate upon reloading was found to be orders of magnitude higher than that prior to unloading. This work addresses observations of recovery responses in Ti-6 wt% Al and Ti-6242 with the variation of several factors including plastic strain level, time spent in the unloaded state, exposure temperature, loading direction, and microstructure. It is proposed that the formation of intense b = <1120> dislocation pile-ups at grain and/or phase boundaries, which stem from the planarity in these alloys, provide the driving force for a thermally activated, dislocation level recovery mechanism.

3:40 PM Break

3:50 PM

Creep of Nearly Lamellar TiAl Alloys Containing 1.0 and 2.0 at.% W: *Andrea Maria Hodge*[1]; Luke M. Hsiung[1]; T. G. Nieh[1]; [1]Lawrence Livermore National Laboratory, Chmst. & Matls. Sci., PO Box 808, L-350, CA 94550 USA

The creep behavior of two nearly lamellar Ti-46.5Al-3.0Nb-2.0W-0.10B and Ti-46.5Al-3.0Nb-1.0W-0.10B (at.%) alloys fabricated by hot-extrusion is investigated as a function of temperature and stress in the low-stress (LS) regime (s<300 MPa). a nearly quadratic (1<n<2) creep behavior was observed for temperatures ranging form 650 to 815°C. The activation energy in the LS regime for the alloy containing 1.0 at.%W was found to be 145.2 kJ/mole. Both the activation energy and the creep exponent values indicate an interface sliding as the dominant creep mechanism at LS regime. The alloy containing 1.0 at.%W performed better than the alloy containing 2.0 at.% W, since the latter contained the weakening b phase.

4:10 PM

A Study of the Oxidation Behavior of the Nb-Ti-Si-Cr-Al-X Alloys: *Raghvendra Tewari*[1]; M. Y. Xu[1]; Hyojin Song[1]; Pablo Rosales[1]; F. J. Boerio[1]; Amit Chaterjee[2]; Vijay K. Vasudevan[1]; [1]University of Cincinnati, Dept. of Chem. & Matls. Engrg., Cincinnati, OH 45221 USA; [2]Rolls Royce Corporation, Indianapolis, IN 46206 USA

Nb-Ti-Si-Cr-Al-X alloys possess attractive properties for structural applications in aero engines. Oxidation properties of these alloys, however, are the matter of concern. The present study addresses the oxidation behavior of these alloys. Specimens of the alloys were exposed to air at a number of temperatures and for various lengths of time and the changes in weight and thickness of the oxide layers monitored. These measurements were coupled with detailed observations of the morphology of the oxide scale, formation of various oxides and the ingress of oxygen into the base materials. Complementary techniques like scanning electron microscopy and x-ray photon spectroscopy have been used to understand the nature and sequences of the oxide scale formation. The role of different alloying elements in the formation of the oxide layer has been critically examined and possible mechanisms of oxidation has been proposed.

4:30 PM

Microstructural Evaluation of LENS™ Deposited Nb-Si Alloys with Varying Ti and Cr Additions: *Ryan Richard Dehoff*[1]; Peter C. Collins[1]; Peter M. Sarosi[1]; Hamish L. Fraser[1]; Michael J. Mills[1]; [1]Ohio State University, Matls. Sci. & Engrg., 2041 College Rd., Columbus, OH 43210 USA

Nb-Si "in-situ" metal ceramic composites consist of Nb_3Si and Nb_5Si_3 intermetallic phases in a body centered cubic Nb solid solution, and show promising potential for elevated temperature structural applications. Cr and Ti have been shown to increase the oxidation resistance and metal loss rate at elevated temperatures compared to the binary Nb-Si system. In this study, the LENS™ (Laser Engineered Net Shaping) process is being implemented to construct the Nb-Ti-Cr-Si alloy system from elemental powder blends due to availability of material and low relative cost. Advantages of the LENS™ process include the ability to produce near net shaped components with graded compositions as well as a more uniform microstructure resulting from the negative enthalpy of mixing associated with the silicide phases. Processing parameters can also be varied, resulting in distinct microstructural differences. Deposits were made with varying compositions of Nb, Ti, Cr and Si. The as-deposited microstructures were examined using SEM and TEM techniques. The influence of composition and subsequent heat treatment on microstructure and mechanical properties will also be discussed.

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Characterization and Aging Studies of New, Cast, High Temperature Aluminum Alloys for Diesel Engine Applications: *Prashanth Prasad*[1]; Yong-Ching Chen[2]; Vijay Vasudevan[1]; [1]University of Cincinnati, Chem. & Matls. Engrg., 2624 Clifton Ave., Cincinnati, OH 45221 USA; [2]Cummins Inc., Metallurgl. Engrg., 1900 McKinley Ave., Columbus, IN 47201 USA

New environmental regulations have placed stringent requirements on emission levels from diesel engines. These requirements can only be met if engines can perform more efficiently, which requires components fabricated from materials that have the required set of mechanical, physical and environmental-resistance properties at elevated temperatures to ~200°C, in combination with low-density and high stiffness. In this context, cast aluminum silicon (354 and 388) alloys are being evaluated, because recent developments at NASA have suggested that with compositional and process modifications, significant enhancement in high temperature strength can result. In this study, the microstructures of cast Al alloys 354 and 388, with and without NASA modification, and in the T5 and T6 conditions were characterized by TEM. In addition, fracture and aging response of these alloys were studied. The results of the structures, compositions and morphology of second phase precipitates, and evolution and mechanisms of precipitation during aging will be reported.

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A Mode Conversion in 2D Surface Pseudoarrays: *Jerzy Kapelewski*[1]; Bogdan Lila[1]; [1]Military University of Technology, Elect. Dept., 2 Gen. Kaliskiego St., Warsaw 00-908 Poland

The purpose of the paper is to outline an unified nonlocal treatment of some mode conversion effects associated with 2D surface pseudoarrays composed of separated regions with varying material parameters. It will be illustrated, in some detail, for the instructive case of a surface acoustic wave (SAW), partly transformed into bulk modes by such a pseudoarray. An analytical model scheme is constructed, using a variational method combined with the T-matrix method, appropriate for the 2D pseudoarray treated, with taking account 3D element profile. An apodization (weighting) to reduce sidelobes level is incorporated into the structure by varying lateral dimensions and depth of particular scatterers. The approach is essentially not restricted to small perturbation of the interface structure, and can be easily extended to allow for near-surface gradient of material parameters, and the effect of a top homogeneous layer.

High Strain Rate Deformation and Deformation Mechanisms of Structural Steels: Deformation Mechanisms and Microstructure Effects

Sponsored by: AIST, AIST - Division VI

Program Organizers: James R. Fekete, General Motors Corporation, Metal Fabricating Division, Pontiac, MI 48341 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA; Benda Yan, Ispat Inland Steel, Product Applications, East Chicago, IN 46312 USA

Monday PM — Room: Grand Ballroom L
September 27, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Benda Yan, Ispat Inland Steel, Product Applications, E. Chicago, IN 46312 USA; James R. Fekete, General Motors Corporation, Metal Fabricating Div., Pontiac, MI 48341 USA

2:00 PM
Microstructure of Adiabatic Shear Bands in a Pre-Shocked 316L Stainless Steel: *Qing Xue*[1]; George T. Gray[1]; Shuh Rong Chen[1]; [1]Los Alamos National Laboratory, Matls. Sci. & Tech. Div., MST-8, G755, Los Alamos, NM 87545 USA

Adiabatic shear localization in a preshocked 316L stainless steel was systematically studied. A forced shear technique on a split-Hopkinson pressure bar was utilized to generate localized deformation on "hat-shaped" specimens. The influence of shock prestraining on shear band microstructural evolution was examined using transmission electron microscopy. Preshocked 316L stainless steel was seen to possess a high density of defects including slip bands, microbands, and deformation twins. The existence of profuse defects and their substructure generated by shock prestraining is seen to lead to a higher susceptibility to shear localization. The shear band width increased with increasing displacement. Elongated subgrains and fine equiaxed subgrains with an average size of 100 nm were observed inside shear bands. The fine subgrains are believed to result from the break-down of the elongated subgrains. Both dynamic and static recoveries are thought to influence the residual shear band substructure; no evidence of dynamic recrystallization or phase transformation was seen.

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Deformation and Shear Band Development in an Ultrahigh Carbon Steel: *Donald R. Lesuer*[1]; Chol K. Syn[2]; Oleg D. Sherby[3]; [1]Lawrence Livermore National Laboratory, L-175, PO Box 808, Livermore, CA 94550 USA; [2]Lawrence Livermore National Laboratory, Livermore, CA 94550 USA; [3]Stanford University, Stanford, CA 94305 USA

Many of the potential applications for ultrahigh carbon steels (UHCS), including products in the automotive and military sectors, involve loading at high strain rates. The mechanical response of a UHCS-1.3C material has been studied at high strain rates (approximately 3000 s-1) with three different microstructures - pearlite, martensite and tempered martensite. Failure for all three microstructures occurred by shear localization. In the pearlitic condition, extensive buckling of the carbide plates was observed and the UHCS-1.3C material exhibited significant potential for compressive ductility (>60%) and energy absorption due to distributed buckling of these plates. Within the shear bands of the pearlitic microstructure, adiabatic heating produced austenite. Subsequent rapid cooling resulted in a divorced eutectoid transformation. The resulting microstructure in the shear band contained nano-scale carbides within ferrite grains and a nanoindentor hardness of 11.5 GPa. The analysis suggests that the divorced eutectoid transformation occurs in hypereutectoid-steel shear bands during high rate deformation resulting from ball milling, ball drop tests and commercial wire drawing. Work performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract No. W-7405-ENG-48.

2:50 PM
Mechanical Response and Constitutive Modeling of Sheet Steels: *Carl M. Cady*[1]; Shuh-Rong Chen[1]; George T. Gray[1]; [1]Los Alamos National Laboratory, MST-8, MS G-755, Los Alamos, NM 87545 USA

The strain rate and temperature sensitivity of the flow stress and the insensitivity of the strain hardening rate indicate that thermal activation over a Peierls barrier is the rate controlling mechanism for many automotive steels. The stress/strain response for the steels is shown to be strongly influenced by strain rate and temperature, which is consistent with this controlling mechanism. Constitutive modeling efforts are able to capture the strain rate sensitivity and work hardening behavior over the range of temperatures and strain rates tested. Based on R-value and texture measurements there is a mild texture as a result of the rolling process. Prestraining raised the yield stress and shifted the flow stress but generally did not change the stress-strain behaviors.

3:15 PM
Dynamic Torsional Properties of Ultra-Fine-Grained Low-Carbon Steels Fabricated by Equal Channel Angular Pressing: *Yang-Gon Kim*[1]; [1]Postech, Dept. of Matls. Sci. & Engrg., San 31, Hyoja-Dong, Nam-Gu, Pohang, Kyungsangbuk-Do 790-784 S. Korea

Dynamic torsional properties of ultra-fine-grained low-carbon steels fabricated by equal channel angular pressing (ECAP) was investigated. Dynamic torsional tests were conducted on four steel specimens, two of which were annealed after ECAP, using a torsional Kolsky bar. The ECAP'ed specimen consisted of very fine, equiaxed grains of 0.2 ìm in size, which were slightly coarsened after annealing. The dynamic torsional test results indicated that maximum shear stress decreased with increasing annealing time, whereas fracture shear strain increased. Some adiabatic shear bands were observed at the gage center of the dynamically deformed torsional specimen. Their width was smaller in the ECAP'ed specimen than in the 1-hr annealed specimen, but they were not found in the 24-hr annealed specimen. These phenomena were explained by dynamic recovery and crystallization due to the highly localized plastic deformation and temperature rise in the adiabatic shear band.

3:40 PM
The Influence of Explosive-Driven Shock Pre-Straining on the Structure/Property Behavior of Copper and 316 L Stainless Steel: *Bulent H. Sencer*[1]; *Stuart A. Maloy*[1]; George T. Gray[1]; [1]Los Alamos National Laboratory, Matls. Sci. & Tech., Grp. MST-8, Struct./Prop. Relations, PO Box 1663, MS G755, Los Alamos, NM 87545 USA

The mechanical response of high-explosive (HE)-driven shock prestrained copper and 316 L stainless steel loaded to 5 GPa has been investigated in compression and tension at room temperature. The microstructure and substructure evolution due to shock pre-straining has been investigated using optical metallography and transmission electron microscopy. The mechanical behavior of 316L stainless steel and Cu following explosive shock pre-straining is shown to exhibit an increase in yield stress and a significant reduction in ductility in tension. Microstructural analyses of Cu revealed cell formation only, while 316L revealed dislocations, planar slip and twin formation. Cu samples shocked with a HE-driven pulse (triangular) show some microstructural differences with those shocked with a and square-top shaped shock pulse loading. In addition, TEM examinations revealed a significant change in the microstructure of Cu after straining at 10-3/s to 5% plastic strain (5% slow strain) compared to that observed in shocked samples (shocked with square-top wave and shocked with triangular wave). These microstructural differences will be explained in detail in this paper and compared to previous results. TEM examinations of 316 L SS revealed significant change in the microstructure of all the samples: 5% slow-strained, square-top wave and triangular wave shock pre-strained samples. All three samples showed a microstructure composed of twinning and dislocations; however twinning seems to be highest in shocked samples. These microstructural differences will be explained in detail in this paper and compared to previous results.

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A Novel Three-Point Bend Test for Dynamic Fracture Toughness Measurement: *Kenneth S. Vecchio*[1]; Jiang Fengchun[1]; Aashish Rohatgi[1]; [1]University of California, Mechl. & Aeros. Engrg., 9500 Gilman Dr., MC-0411, La Jolla, CA 92093-0411 USA

A modified split Hopkinson pressure bar loaded impact test, referred to as a two-bar/three-point bend test (with a momentum trap), has been developed to measure dynamic fracture toughness. In this paper, we summarized some theoretical and experimental work conducted on this novel dynamic fracture experimental technique. The loading principle and advantages of this setup are introduced, and then the effect of support motion (transmission bar) on sample's deflection was analyzed theoretically and experimentally. The result indicated that the effect of support motion is very small and can be neglected, and it is only necessary to compute the dynamic load applied on sample using one-dimension stress wave theory. In order to measure dynamic fracture toughness, a simple formula of dynamic stress intensity factor for a pre-cracked three-point bend specimen is derived using the vibration analysis method. Here, shear deformation and rotary inertia was introduced into the calculation of the dynamic stress intensity factor by means of solving the stiffness of a pre-cracked three-point bend specimen. This technique has been validated for several high-strength structural steels of varying fracture toughness. The dynamic fracture initiation toughness was measured using this technique, and the fracture micro-characteristics of the stretch zone were documented in each case. Two different crack initiation mechanisms, i.e., of brittle (quasi-cleavage) and ductile (microvoid coalescence) were observed and correlated with the sample's mechanical response as determined by this novel dynamic fracture test. This is possible because a single compression pulse loads the sample, without being subjected to any additional reflected pulses due to the use of a momentum trap.

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High Speed Deformation Behaviour of a Dual Phase Steel: *Jinbo Qu*[1]; Steve Yue[1]; [1]McGill University, Dept. of Mining, Metals & Matls., M.H. Wong Bldg., 3610 Univ., Montreal, Quebec H3A 2B2 Canada

By means of dynamic Hopkinson bar shear punch testing, the high-speed deformation behaviour of dual phase steel was studied, with an emphasis on the influence of microstructure. Dual phase microstructures with different fractions of martensite, acicular ferrite, and bainitic microstructure were obtained by changing heat treatment parameters during intercritical annealing. Quasi-static shear punch properties were also measured by MTS hydraulic machine and compared with dynamic results. Standard tensile tests for some specimens were conducted for comparison.

5:10 PM
Plastic Deformation and Fracture of Steels Under Dynamic Biaxial Loading: *Chol K. Syn*[1]; Juan C. Moreno[1]; Dana M. Goto[1]; James F. Belak[1]; Dennis E. Grady[2]; [1]Lawrence Livermore National Laboratory, PO Box 808, Livermore, CA 94551 USA; [2]Applied Research Associates, 4300 San Mateo Blvd. NE, Albuquerque, NM 87110 USA

A novel gas-gun experiment is used to study dynamic deformation and fracture under biaxial loading condition. A small copper projectile impacts a thick copper plate on which a thin steel target plate is mounted. The thickness of the flyer is chosen to produce a spall plane at the copper-steel interface. In the velocity range of 1-2 km/s, the steel target is observed to first bulge, then form incipient fractures, and finally to fracture open in a petalled pattern. The targets were soft captured in light foam. In a variation of the target geometry, curved steel targets with a constant radius of curvature are used with copper plate with the matching curvature. AerMet 100 with and without the hardening heat treatment and hot-rolled 1010 steel were used as target materials. Results will be presented for the strain-to-failure and the microscopic structure of the incipient fractures. Concurrently, the simulation code, CALE, was used to analyze the stress history during the experiment. This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

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Influence of Prestraining and Microstructure on the Dynamic Properties of High Strength Sheet Steels: *Patrick Larour*[1]; Mathieu Prigent[2]; Manuel Antonio Real Gomes[3]; Andreas Wedemeier[4]; Jean-Luc Jeoffroy[5]; [1]University of Aachen, Dept. of Ferrous Metall., Intzestrasse 1, Aachen D-52072 Germany; [2]OCAS-ARCELOR, R&D, John Kennedylaan 3, Zelzate B-9060 Belgium; [3]ISQ Instituto de Soldadura e Qualidade, LABMech Lab., Apartado 119 Tagus Park, Oeiras P-2781-951 Portugal; [4]Salzgitter Mannesmann Forschungszentrum, Werkstoffzentrum, Eisenhüttenstraße 99, Salzgitter D-38239 Germany; [5]LEDEPP-ARCELOR, R&D, 17 ave. des Tilleuls, Florange F- 57190 France

The influence of pre-straining and microstructure on the dynamic properties of car body high strength steels has been investigated taking into account the influence of strain rate at room temperature. The mechanical properties of a dual phase DP600, a TRIP700 and an austenitic steel 1.4318 have been determined performing high speed tensile tests and Split-Hopkinson bar tests using flat sheet samples in the strain rate range from 0.005s-1 to 950s-1. Uniaxial, biaxial and plane strain pre-straining modes have been investigated and compared to the as-delivered material. Microstructure and fractography analysis have been performed. Furthermore this conference paper also focuses on the influence of specific test requirements for dynamic tensile and Split-Hopkinson bar testings of thin sheet steels.

Materials Damage Prognosis: Integrated Health Management

Sponsored by: TMS - Structural Materials Division
Program Organizers: James M. Larsen, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson AFB, OH 45433-7817 USA; Jeffrey R. Calcaterra, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson Air Force Base, OH 45433-7817 USA; Leo Christodoulou, Defense Advanced Research Agency, Arlington, VA 22203-1714 USA; Michael L. Dent, Anteon Corporation USA; William J. Hardman, Naval Air Systems Command, Propulsion and Power Directorate (AIR 4.4.2), Patuxent River, MD 20670-1534 USA; Paul Hoffman, United States Navy, NAVAIR, Patuxent River, MD 20670 USA; J. Wayne Jones, University of Michigan, College of Engineering, Department of Materials, Science and Engineering, Ann Arbor, MI 48109 USA; Stephan M. Russ, Air Force Research Laboratory, Materials and Manufacturing Directorate, AFRL/MLLN, Wright-Patterson Air Force Base, OH 45433-7817 USA

Monday PM — Room: La Galerie 6
September 27, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Mark M. Derriso, Air Force Research Laboratory, VASA, Wright Patterson AFB, OH 45433 USA; Kumar V. Jata, Air Force Research Laboratory, Wright Patterson AFB, OH 45433 USA

2:00 PM Invited
Integrated Systems Health Management: Enabling Technology for Effective Utilization of Weapon Systems: *Mark M. Derriso*[1]; [1]Air Force Research Laboratory, VASA, 2790 D. St., WPAFB, OH 45433 USA

The Department of Defense (DoD) is currently evaluating different methodologies to reduce cost, increase availability and maintain safety of current and future weapon systems. As the DoD aircraft increases in age, so does its operating and support (O&S) cost. One of the biggest cost drivers in the fleet today is due to unscheduled maintenance. Because the average age of DoD's aircraft is roughly 25 years old, more inspections are being performed to maintain safety, which results in a decrease in fleet availability. DoD has implemented a new policy call "Conditioned-Based Maintenance Plus" (CBM+) in an attempt to improve the current aircraft maintenance procedures. Just as the title indicates, DoD wants to migrate to a process that performs maintenance based on the current condition of the vehicle instead of the current schedule-based approach. The current paper describes how Integrated Systems Health Management (ISHM) is critical for implementing CBM. ISHM will enable DoD to meet its objectives of improving maintenance agility and responsiveness, increasing operational availability, and reducing life cycle total ownership cost.

2:25 PM Invited
An Advanced COTS System Health Management Solution: *Kevin Cavanaugh*[1]; [1]Qualtech Systems, Inc.

The briefing will introduce Qualtech Systems, Inc. (QSI) and the TEAMS (Testability Engineering and Maintenance System) solution. QSI has a wealth of experience designing and implementing advanced, intelligent health management solutions with NASA, Sikorsky Helicopter, Honeywell, Boeing, Pratt & Whitney, US Navy, US Air Force, and US Army. The technology, currently being implemented on Army UH-60 Blackhawk, AH-64D Apache, and S-92 Helicopters, includes on-board diagnostics, intelligent debrief, dynamic/optimized IETM, reasoner driven test equipment, and remote health management (or Telemaintenance). The TEAMS tool set provides system "failure behavior" graphical modeling, rigorous diagnostics (testability) analysis, embedded run-time diagnostics, drives support equipment with intelligent reasoning, serves intelligent/dynamic maintenance procedures, and can be implemented in a large-scale server for networked remote diagnostics and health management. The briefing will describe these capabilities and give examples of current real world applications and the value (operational and cost) attributed to the TEAMS technology. The overall solution generates a diagnostic knowledge base; manages models, diagnostic logs, and health related data; and employs model-based reasoning to process fault signatures for rapid/accurate diagnosis.

2:50 PM Invited
Framework for Testing Prognosis Technology: *Bruno J. Jambor*[1]; [1]Lockheed Martin Space Systems, PO Box 170, Denver, CO 80201 USA

This paper describes a framework for testing prognosis technology in complex mechanical subsystems. The framework uses commercial off-the-shelf hardware and software to test subsystems in a hardware-in-the-loop realistic environment. The framework allows testing the constitutive elements of the prognosis technology: data acquisition, data structuring, preprocessing, and production of prognosis results. The paper considers the interactions between prognosis algorithm complexity, real time execution requirements, and integration into a real-time architecture where the control and prognosis functionalities cooperate to allow timely decision-making. The paper also considers the requirements for including the prognosis results into a maintenance and operations decision and logistics support system. Applications described include flight surface actuators and thermal protection systems. The paper covers methods for modeling and simulation, data management, data fusion, and automation of task execution.

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Health Management System Architecture for Integrated System-Wide Analysis: *Renee M. Kent*[1]; Anthony Bartolini[1]; Thomas E. Munns[1]; [1]ARINC Engineering Services, Annapolis, MD USA

Our work entails the development of a reasoning infrastructure that fuses information from multiple, multi-variate sources, including operation and sensor data, to identify, characterize, isolate, and predict specified faults at the system-level of a complex system or subsystem. Consideration is given to fusion of a variety of disparate information sources, sensors, and models for identification of faults in a multi-fault environment. The basis of this work incorporates a novel distributed reasoning architecture, in which constraints of processing in a real-time onboard environment are considered and in which adaptive domains can be incorporated for expandability to allow for increases in task complexity. Our system has been integrated onto an aircraft for demonstration of the onboard health management capability. In this presentation, we will present results from recent research on the application of this approach to on-aircraft health management.

3:50 PM

A Dynamical Systems Engineering Approach to Vehicle Health Monitoring and Nondestructive Inspection System Design: *William G. Frazier*[1]; Danny L. Parker[1]; [1]Miltec Research and Technology, Inc., 9 Industrial Park Dr., Oxford, MS 38655 USA

Research and development of sensor technologies for vehicle health monitoring and imbedded nondestructive testing continues and new technologies are emerging. As a result, the need for strategies for designing comprehensive systems for vehicular (aircraft or ground vehicles) systems has become even greater. Primary questions such as what kind of health problems are expected and how rapidly will they develop, what kinds of sensors should be used, how many of each kind should be used, where should they be placed, and how should the data be processed, arise. In order to make the most of new sensors and signal processing technologies, monitoring and inspection systems should be designed with all of the above questions (and others) concurrently in mind, and not just sequentially. Approaches that are capable, in principle, of addressing these issues; i.e. those based upon dynamical systems engineering, are being investigated. Briefly stated, dynamical systems engineering provides a systematic framework for system design that is based primarily on the use of integrated, comprehensive models of cause and effect. For example, using state-of-the-art multi-scale models that relate fatigue damage to dynamic behaviors (vibration/acoustic, magnetic, etc.) for a component or assembly of components, it is feasible to determine optimal sensor placement to achieve maximum likelihood of detecting damage development. Moreover, the techniques extend to damage estimation (diagnosis) and prediction (prognosis) using principles from random process theory, and they can also be used to help solve inverse problems such as what sensor capability is required (specification determination) in order to achieve reasonable performance goals. Our presentation will focus on how dynamical systems engineering is being used by us and others to address design problems in IVHM and NDI. Experimental results for particular applications will also be presented.

4:15 PM Invited

Built-in Diagnostic Imaging for Structures: *Fu-Kuo Chang*[1]; [1]Stanford University, Dept. of Aeronautics & Astronautics, Stanford, CA 94305 USA

Although recent advances in structural health monitoring (SHM) technology have demonstrated the feasibility of detecting and locating damage in complex structures based on sensor measurements, qualifying the damage based on sensor measurements still remains a challenging task. A digital imaging technique based on a time-reversal concept has been developed for qualitative monitoring of damages in structures. The proposed technique utilizes signal processing, beamforming based algorithms, and distributed sensor/actuator networks to produce an image of structural damage. The resolution of the image may also depend on the density and the location of sensors and actuators. The technique requires information about specific propagating group velocities which need to be determined by either analysis or experiment. As an alternative, an auto-focusing method gene rating a self-focused image is proposed to demonstrate the feasibility of a technique requiring no group velocity information. Experimental results on an aluminum plate and a composite sandwich panel show that the imaging technique using built-in piezoelectric actuator/sensors can monitor crack and delamination damage in terms of location and approximate size. Also shown is that detailed damage information such as crack orientation and progressive change can be identified from the resulting image.

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Method and System for Discovering and Recovering Unused Service Life: *Stephen V. Zaat*[1]; [1]Boeing Company, Network Centric Ops., Phantom Works, PO Box 516, MC S111-1335, St. Louis, MO 63166-0516 USA

Owners of aircraft, such as the military, face a dilemma of trading off between the cost of new replacement aircraft and the cost of modernization and upgrades to existing aircraft. Modernization and upgrades are generally less expensive than new aircraft, but can be financially justified when sufficient service life remains in an aircraft. Traditional methods employed for determining service life expended and service life remaining are based solely upon cumulative flight hours and load assumptions. For aircraft flown under less demanding conditions than predicted, actual aircraft service life can be significantly greater than the determined service life when designed. When modernizations and upgrades are considered for older aircraft, fatigue testing is used to determine service life remaining. Fatigue testing is destructive, very expensive, and time consuming. Therefore, there exists an unmet need to non-destructively determine service life in a less costly way.

Modeling and Computer Applications in Metal Casting, Shaping & Forming Processes: Modeling and Computer Simulation: Tube Making and Related Processes

Sponsored by: AIST, TMS - Extraction & Processing Division, TMS - Materials Processing & Manufacturing Division, TMS, TMS - MPMD/EPD-Process Modeling Analysis & Control Committee, TMS - MPMD-Shaping and Forming Committee, TMS - MPMD-Solidification Committee, AIST - Division VI, AIST - Division VII, TMS - MPMD-Computational Materials Science & Engineering-(Jt. ASM-MSCTS)
Program Organizers: Krich Sawamiphakdi, The Timken Company, R&D Manufacturing Technology, Canton, OH 44706 USA; Praveen Pauskar, The Timken Company, Advanced Process Technology, Timken Research, Canton, OH USA; Maciej Pietrzyk, Akademia Gorniczo-Hutnicza, Department of Computer Methods in Metallurgy, Krakow Poland; Raghavan Srinivasan, Wright State University, Department of Mechanical & Materials Engineering, Dayton, OH 45435 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA; Brian G. Thomas, University of Illinois, Department of Mechanical and Industrial Engineering, Urbana, IL 61801 USA

Monday PM Room: La Galerie 2
September 27, 2004 Location: Marriott New Orleans Hotel

Session Chairs: Praveen M. Pauskar, The Timken Company, Advd. Process Tech., Canton, OH 44706-0930 USA; Mohammed Maniruzzaman, Worchester Polytechnic Institute, Worchester, MA 01609-2280 USA

2:00 PM

Tube Optimization Model: An Integrated Process Modeling and Optimization Tool for Seamless Tubemaking: *Daqing Jin*[1]; Jeffery E. Ives[1]; E. Buddy Damm[1]; Anthony J. Perez[1]; Krich Sawamiphakdi[1]; [1]The Timken Company, Canton, OH 44718 USA

An integrated process modeling and optimization tool - Tube Optimization Model (TOM) was developed for the simulation of thermal, mechanical and microstructural evolution during the seamless tube-making process. Process mathematical models were developed at The Timken Company and in cooperation with external partners to analyze the entire tube making process including: piercing, Assel elongating, reducing, stretch-reducing, induction heating, rapid cooling, and annealing. In addition, metallurgical models for recrystallization, grain growth, transformation and flow stress for numerous steel grades have been developed and integrated. The finite-element and finite-difference approaches were employed in the mathematical models. The tool enables the engineers at Timken to design the controlled thermal mechanical processing paths for tube making to tailor the customer's demands on mechanical properties, formability and machinability in conjunction with reductions in the energy and processing costs. Selected case studies will be presented to illustrate the utility of TOM. Timken completed this work with partial funding award from the U.S. Department of Energy.

2:25 PM

Improvement of Surface Finish in Steel Hot Rolling by Optimal Cooling Ahead of Entry into the Roll Gap: Numerical Analysis: *Michal Krzyzanowski*[1]; John H. Beynon[1]; [1]University of Sheffield, Dept. of Engrg. Matls. (IMMPETUS), Sir Robert Hadfield Bldg., Mappin St., Sheffield, S. Yorkshire S1 3JD UK

Numerical analysis based on the finite element method allowed evaluation of optimal cooling conditions at entry into the roll gap with the aim of improvement of the product surface finish in hot rolling of steel by decrease of scale related defects. Influence of surface cooling just before the roll gap on descalability of secondary oxide scales was under the investigation. Several phenomena were considered, such as elastic-plastic deformation, viscous sliding along the oxide metal interface, thermal expansion/contraction of the oxide/metal system and also cracking and spallation of the oxide scale from the metal surface. A water spray impact was simulated as transient boundary conditions for pressure and heat transfer on the basis of available results of experimental investigations and theoretical assumptions of hydraulic descaling. Calculation of the tangential viscous sliding, which arise from the shear stresses transmitted from the steel to the scale, was based on a microscopic model for stress-directed diffusion around irregularities at the interface and depends on the temperature, the interface roughness parameters, the volume-diffusion coefficient and the diffusion coefficient for metal atoms along the oxide/metal interface. Cracking of the scale was allowed to occur along the surface of lowest energy release rate on the basis of the J-integral calculation. Maintaining the optimal temperature at the surface layer ahead of entry into the roll gap allowed for the production of either a crack-free oxidized metal surface or increased descalability of the cracked oxide scale. The temperature distribution depends on the steel composition, scale thickness and other rolling parameters.

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Analysis of Variation of the Mean Wall Thickness in Stretch Reduced Tubes: Gennady I. Gulyayev[2]; Yury G. Gulyayev[3]; Yevgeny I. Shyfrin[4]; Nataliya Yu. Kvitka[5]; *Krich Sawamiphakdi*[1]; [1]The Timken Company, Timken Rsch., 1835 Dueber Ave. SW, PO Box 6930, Canton, OH 44706-0930 USA; [2]Osada State Tube Institute (DTI-VNITI), Dniepropetrovsk, 49600 Ukraine; [3]Nizhnieprovsky, Dniepropetrovsk, 49064 Ukraine; [4]Nizhniednieprovsky Tube Works (NTZ), Dniepropetrovsk, 49064 Ukraine; [5]National Metallurgical Academy of Ukraine, Dniepropetrovsk, 49005 Ukraine

The proposed mathematical model determines the variation of the mean wall thickness in stretch reduced tubes based on variational principles of plastic metal working characteristics. The model takes into account influence of mechanical characteristics, namely yield strength and hardening behavior of the deformed material on the pattern of the wall thickness variation. The general mathematical model also considers the influence of contact conditions, amount of deformation and rheological conditions between rolls and mother tubes on the mean wall thickness variation during the forming process. The analysis of deformed energy balance enables the proposed generalized mathematical model to determine the changes in the mean wall thickness in the stretch reducing mill. The comparison of calculated and experimental data is presented in the paper to confirm the accuracy of the proposed model.

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Overview of 3D Finite Element Modeling in Tube Making Processes at the Timken Company: *Krich Sawamiphakdi*[1]; Daqing Jin[1]; Anthony J. Perez[1]; [1]The Timken Company, Canton, OH 44706 USA

At The Timken Company, finite element modeling has been utilized successfully to design, improve and optimize metal-forming processes in many areas including steel-making processes for long products and tubes, and forming and shaping of discrete parts. It is very challenging to apply the finite element modeling to the tube making processes due to continuously changing contact conditions between the workpiece and forming tools. This paper illustrates the use of different finite element formulations for the analysis of various tube making processes in the plant. As a result of the differences between finite element analysis (FEA) programs, utilization of the most suitable program to analyze a certain process can be quite significant. Program selection as well as analysis results of several cases are presented in the paper to demonstrate the proper utilization of each FEA program. Excellent agreement between predicted and in-plant data was observed. This work has been done by Timken under a partial funding award from the U.S. Department of Energy.

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Application of Computer Programs to Assist the Tooling Design for the Skew Rolling Process: *Ming He*[1]; Krich Sawamiphakdi[1]; [1]The Timken Company, Canton, OH 44706 USA

Conventional approach of the tooling design in the skew rolling process is based on the designers' experience and trial and error, which requires a number of design iterations and tests. The tests are generally expensive and time consuming that leads to a long lead-time to market. Application of the finite element analysis as an extended design tool in the process allows designers to evaluate, validate and optimize the design before the tooling is actually made. The simulation results make it possible to gain an insight of initiation of root problems, to study their influence on product quality, to reduce design lead-time and to increase cost effectiveness. The paper will describe the development of the analysis programs to assist the tooling design for the skew rolling process.

4:15 PM

Accurate Temperature Measurement During Water Quench Operations: Dianfeng Li[1]; *Mary Wells*[1]; Steve Cockcroft[1]; [1]University of British Columbia, Metals & Matls. Engrg., 309-6350 Stores Rd., Vancouver, BC V6T 1Z4 Canada

A critical aspect of process control in industry is the development of representative mathematical models that can be used to optimize the operation in either an off-line or real-time mode. Inherent to the accuracy of the model predictions is precise knowledge of the boundary conditions in the process. In situations where water quenching is used to control the temperature of the product being produced, it is important to understand quantitatively the heat transfer at the surface of the product during the quench operation; typically this is done using a boiling water curve. Often these boiling curves are determined by using experimental measurements of temperature-time data in the product during a quench operation in conjunction with Inverse Heat Conduction (IHC) models. The experimental data used are usually measured using thermocouples installed in the sample being cooled at a known sub-surface location. This paper outlines the errors associated with using sub-surface thermocouples during a water quench operation characterized by boiling water heat transfer. The study showed that, during severe quench tests where the heat flux was very high, the hole used to install the thermocouple had to be included in the analysis in order to obtain the accurate temperature-time data and, hence, boiling curves. This work has been performed at the request of The Timken Company under a partial funding award from the U.S. Department of Energy.

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Process Modeling for Rotary Tube Piercing Application: *Jaebong Yang*[1]; Guoji Li[1]; Wei-Tsu Wu[1]; Krich Sawamiphakdi[2]; Daqing Jin[2]; [1]Scientific Forming Technologies Corporation, Columbus, OH USA; [2]The Timken Company, Canton, OH 44706 USA

Rotary piercing of a solid rod into a seamless tube, also known as the Mannesmann process, is a very fast rolling process. In the process, the process cross rolls the preheated billet between two barrel-shaped rolls at a high speed. Driven by the cross rolls, the workpiece rotates. High tensile stresses occurs at the center of the billet. The material starts to split at the tip of the plug and to form the tube shell. To study the rotary piercing process, the Finite Element Method (FEM) based commercial code DEFORM was used. The updated Lagarangian approach was first used in the investigation. Excellent agreement between the numerical prediction and actual part shape was observed. Due to the dominated rotational velocity field, the time step size is limited to a small value and complete part must be modeled for better solution accuracy. It therefore increases the computing effort. To reduce the CPU time, a new method with the Eularian approach was developed. The geometry updating is carried out in the feeding direction while the hoop direction remains unchanged. Using this approach, only a portion of the model is needed due to the symmetry condition. This paper summarizes the overall methodologies. A tube piercing process was presented to demonstrate the technique.

Pb-Free and Pb-Bearing Solders: Session II

Sponsored by: TMS - Electronic, Magnetic & Photonic Materials Division, EMPMD-Electronic Packaging and Interconnection Materials Committee
Program Organizers: C. Robert Kao, National Central University, Department of Chemical and Materials Engineering, Chungli City 32054 Taiwan; W. Plumbridge, Open University, School of Engineering Materials, Milton Keynes MK7 6AA UK; K. N. Subramanian, Michigan State University, Chemical Engineering & Material Science, East Lansing, MI 48824 USA

Monday PM — Room: Grand Ballroom K
September 27, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: John William Morris, Jr., University of California, Dept. of Matls. Sci. & Engrg., Berkeley, CA 94720 USA; Kwang-Lung Lin, National Cheng Kung University, Dept. of Matls. Sci. & Engrg., Tainan Taiwan

2:00 PM Invited
Next Generation of Lead-Free Solders: Low Temperature Solders: *Katsuaki Suganuma*[1]; [1]Osaka University, Inst. of Scientific & Indust. Rsch., Mihogaoka 8-1, Ibaraki, Osaka 567-0047 Japan

Lowering soldering temperature besides the expansion of new Sn-Ag-Cu standard lead-free alloy has been emerged as one of the key issues in establishing lead-free mounting technology. One can select Sn-Zn alloys with or without third alloying elements, Sn-Ag-In alloys and Sn-Bi eutectic alloys. Each has its own benefits and drawbacks and one must keep them in consideration when they will adopt these low temperature solders. As for Sn-Zn alloys, the stabilities of the inetrafce with Cu substrate at elevated temperatures and in humid atmosphere are our main concern. Diffusion of Zn and Cu in Sn matrix has a key role and alloying elements such as Al and Ti have some influence on the degradation behavior. The addition of In to Sn-Ag alloy modifies the dispersion of fine intermetallic compounds from Ag3Sn to Ag3In beyond about 3 wt% In. In pllying these low temperature solders, one needs to note the formation of extremely low temperature melting reaction, especially in the presence of Pb contamination, that frequently occur near joint interfaces resulting in detrimental interface effects.

2:30 PM Invited
Dissolution Behavior and Interfacial Morphology of Cu and Ag in Reacting with Molten Lead-Free Solders: *Kwang-Lung Lin*[1]; Po-Yi Yeh[1]; Jenn-Ming Song[1]; [1]National Cheng Kung University, Matls. Sci. & Engrg., 1 Ta-Hsuey Rd., Tainan 701 Taiwan

This study investigated the dissolution behavior, at 300~400°C, of Cu and Ag in molten Sn-4.0Ag-0.5Cu (abbreviated as Sn-Ag-Cu), Sn-8.6Zn (abbreviated as Sn-Zn) lead-free solders, as well as that in Sn-37Pb (abbreviated as Sn-Pb) eutectic solder. Results show that the dissolution rate was significantly lower and the activation energy of dissolution was higher for both the Cu and Ag in molten Sn-Zn eutectic solder than in Sn-Pb and Sn-Ag-Cu. Cu exhibited the greater dissolution rate in molten Sn-Ag-Cu solder than in any other solders, while the Ag dissolves faster in Sn-Pb solder than in others. Interfacial intermetallics and their morphology govern the dissolution behavior. In the case of Sn-Pb and Sn-Ag-Cu solders, whisker Cu-Sn and Ag-Sn compounds formed at the interface with Cu and Ag substrates, respectively. On the other hand, layer Cu-Zn and Ag-Zn were detected at the interface of Sn-Zn/Cu and Sn-Zn/Ag. The Ag-Zn intermetallics became discrete at the temperature of 350°C or above and led to a subsequent high dissolution rate for Ag in Sn-Zn.

3:00 PM
Interfacial Reactions in Sn-Rich Solders: *John William Morris*[1]; Kyu Oh Lee[1]; Jamie Tran[1]; Fay Hua[2]; [1]University of California, Matls. Sci. & Engrg., 210 Hearst Mining Bldg., Berkeley, CA 94720 USA; [2]Intel Corporation, Sunnyvale, CA USA

The authors report further studies of the development of intermetallics at interfaces between Sn and Cu and Sn and Ni|Au. Prior work has shown the development of an extensive intermetallic at the Sn-Ni|Au interface in Sn-rich solders with the asymmetric metallization Cu||Sn||Au|Ni. The extensive intermetallic apparently influences the solder creep rate, and may influence other mechanical properties. We discuss the composition, mechanism of formation and consequences of the intermetallic layer.

3:25 PM
Morphology and Size Distribution of Cu6Sn5 Scallops as a Function of Composition of SnPb Solder: *Jong-ook Suh*[1]; Andriy M. Gusak[2]; King-Ning Tu[1]; [1]University of California, Matls. Sci. & Engrg., Los Angeles, CA 90095-1595 USA; [2]Cherkasy State University, Theoretical Physics, Cherkasy Ukraine

In flip chip technology, spalling of intermetallic compound at the interface between solder and thin film under-bump-metallization is an important reliability issue. The origin of spalling is the consumption of metal thin film due to solder reaction, in which the growth of the scallop-type intermetallic compound is accompanied by ripening. A kinetic model of the non-conservative ripening has been presented by Gusak and Tu (Phys. Rev. B66, 115403, 2002). To compare the model with experimental observations, the size distribution of scallops as a function of SnPb solder composition on copper has been study. Influence of the solder composition on Cu6Sn5 morphology was investigated first to obtain reproducible scallop-like intermetallic compound at the interface. Then, the time dependence of size distribution and average grain size of Cu6Sn5 was measured. The results will be presented.

3:50 PM Break

4:05 PM Invited
The NEMI Sn-Ag-Cu Solder Alloy: A Review of its Nature and Factors that Affect its Microstructure: *D. D. Perovic*[1]; L. Snugovsky[1]; J. W. Rutter[1]; [1]University of Toronto, Ctr. for Microelect. Assembly & Pkgg., Dept. of Matls. Sci. & Engrg., Toronto M5S 3E4 Canada

The NEMI Pb-free (Sn-3.8 wt.% Ag-0.7 wt.% Cu) alloy has a near ternary eutectic composition and on freezing forms a faceting lamellar Ag3Sn phase and a faceting fibrous Cu6Sn5 phase in a nonfaceting Sn matrix. The usual cast microstructure consists of Sn dendrites with interdendritic eutectic. The equilibrium solid solubilities of Ag (0.04 wt%) and Cu (0.0063 wt%) in Sn are very low, so that the matrix phase is nearly pure Sn. With increasing cooling rate, the volume fraction of Sn dendrites increases, so that the interdendritic "eutectic" correspondingly contains increasing amounts of Ag (as Ag3Sn) and Cu (as Cu6Sn5). The formation of a dendritic microstructure results in interdendritic shrinkage on freezing, producing a rough cast surface, which is of importance in visual inspection of soldered joints. Because the alloy composition is off eutectic, Ag3Sn should be, and usually is, the primary phase on solidification. However, growth of Ag3Sn can lead to nucleation of Sn dendrites, as a result of a constitutional undercooling phenomenon. Under some freezing conditions, Sn can form the primary phase. On ageing at 150°C, rapid alteration of the cast microstructure occurs. Coarsening of the Cu6Sn5 phase is most rapid, due to the extremely fast diffusion rate of Cu in solid Sn. Ag3Sn coarsens more slowly. The coarsening occurs by the Ostwald ripening mechanism.

4:35 PM Invited
Study of Oxidation of Sn Alloys for Microelectronic Applications: *Sungil Cho*[1]; Jin Yu[1]; Sung K. Kang[2]; Da-Yuan Shih[2]; [1]KAIST (Korea Advanced Institute of Science and Technology), Dept. Matls. Sci. & Engrg., CEPM, 373-1 Gusung-dong, Yusung-gu, Daejon 305-701 S. Korea; [2]IBM T.J. Watson Research Center, Yorktown Heights, NY 10598 USA

Most metal tends to form surface oxides spontaneously under ambient or aqueous condition. The presence of oxides on the surface of solder alloys used in microelectronic applications is of critical importance. It affects the formation of otherwise a good solder joint by degrading their solderability and the mechanical reliability of solder joints. The solid-state oxidation of pure Sn (electroplated and cast/rolled), high Pb-Sn alloys and eutectic 63Sn-37Pb solder was studied by using an electrochemical oxide reduction method. The oxidation conditions applied were at elevated temperatures in dry air and under a humid condition. Both the type and the amount of oxides were measured quantitatively. It was also observed that a low valence Sn oxide transformed to a high valence Sn oxide during oxidation. To investigate the effect of Cu on Sn oxidation in Pb-free solder applications, the oxidation behavior of electroplated Sn on Cu metallization was also investigated.

5:05 PM
Microstructural Evolution Leading to Brittle Fracture in the Pb-Free Sn-4.0Ag-0.5Cu Ball Grid Array Solder Sphere Alloy: *Daniel Cavasin*[1]; Robert Zheng[2]; [1]Advanced Micro Devices, PCSG, 5204 E. Ben White Blvd., MS PCS-3, Austin, TX 78741 USA; [2]Advanced Semiconductor Engineering, Inc., QA, 25 Chin 3rd Rd., Kaohsiung 811 Taiwan

Failure analyses were conducted on various Ball Grid Array (BGA) packages which failed in reliability testing due to solder sphere separation. The sphere alloy was Sn-4.0Ag-0.5Cu, while the BGA substrate pad finish consisted of electrolytic Ni/autocatalytic Au plating. Reliability testing included multiple reflows at the JEDEC MSL3/260C standard condition, as well as High Temperature Storage (HTS) and Temperature Cycling (T/C). Examination of the separated interfaces indicated a brittle fracture mode. Elemental analyses indicated the presence of a Ni-Sn intermetallic compound adhering to the substrate pad surface, while the surface of the detached material showed the presence of both ternary and quaternary Sn-based intermetallic compounds. A comparison was made between the thermal history of the failed units and microstructure evolution studies which had correlated joint strength degradation and intermetallic layer growth to time/temperature conditions. Results confirmed that the brittle fracture mode was the result of the formation and subsequent cleavage of two distinct Ni-Sn based intermetallic compounds.

Precipitation in Steels - Physical Metallurgy and Property Development: Phase Transformation

Sponsored by: AIST, AIST - Division V, AIST - Division VI
Program Organizers: Luis Ruiz-Aparicio, Duferco Farrell Corporation, Farrell, PA 16121 USA; Dengqi Bai, IPSCO Inc., Muscatine, IA 52761 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Monday PM — Room: La Galerie 3
September 27, 2004 — Location: Marriott New Orleans Hotel

Session Chair: Stephen Yue, McGill University, Dept. of Metals & Matls. Engrg., Montreal, Quebec H2X 3R2 Canada

2:00 PM
Dilatometric Investigations on the Decomposition of Austenite in Two Medium-Carbon Steels Respectively With and Without Cr and Mo Additions: *Anne Isabelle Mertens*[1]; Lie Zhao[2]; Andrew Brown[3]; Joseph McDermid[1]; Jilt Sietsma[4]; Sybrand van der Zwaag[5]; [1]McMaster University, Mechl. Engrg., Main St. W., 1280, Hamilton, Ontario L8S 4L7 Canada; [2]Netherlands Institute for Metals Research, Rotterdamseweg, 137, Delft 2628AL The Netherlands; [3]University of Sheffield, Engrg. Matls., Sir Robert Hadfield Bldg., Mappin St., Sheffield S1 3JD UK; [4]Delft University of Technology, Matls. Sci. & Engrg., Rotterdamseweg, 137, Delft 2628AL The Netherlands; [5]Delft University of Technology, Aeros. Engrg., Kluyverweg, 1, Delft 2629HS The Netherlands

The interest of small additions of Cr (< 3 wt %) and Mo (~ 0.2 wt %) in steels for automotive and bearing applications has been recently highlighted. The microstructure of these steels is primarily based on the bainitic phase. Therefore, in order to optimize their microstructure and their mechanical properties, it is of primary importance to gain a better understanding of the influence of Cr and Mo on austenite decomposition in varying temperature regimes with a particular attention to the transition between ferrite, bainite and martensite formation. In the present work, dilatometry, combined with detailed microstructural characterisation, is used in order to obtain a full view of transformation processes and kinetics in two medium-carbon steels, respectively with and without Cr and Mo additions.

2:25 PM
Ferrite Nucleation on Ce-Oxysulphide Inclusions in Low Alloyed Steels: *Casper Van der Eijk*[1]; Ilkka Lassila[2]; Øystein Grong[3]; Ole Svein Klevan[4]; Lauri Holappa[2]; [1]SINTEF, Matls. & Chmst., R. Birkelands vei 3a, Trondheim N-7465 Norway; [2]Helsinki University of Technology, Lab. of Metall., Espoo FIN-02150 Finland; [3]Norwegian University of Science and Technology, Dept. of Matls. Tech. & Electrochmst., Trondheim N-7491 Norway; [4]Elkem GmbH, PO Box 2455, Meerbusch D-40647 Germany

The concept of intragranular ferrite nucleation by specific inclusions is well known from steel weld metals. In this work, it is shown that the idea can be transferred to steel metallurgy. The paper describes lab-scale experiments in which a Ce-containing alloy and an alloy containing a fine dispersion of MnS inclusions were added to liquid low alloy steel and cast immediately after these alloying additions. This is done in order to create a large number of small Ce-oxysulphide inclusions which are capable of nucleating acicular ferrite. The experimental steels were then subjected to thermal simulation at peak temperatures and cooling programs, similar to those encountered during welding. The steels containing Ce-oxysulphide inclusions with MnS on their surface appear to contain a high amount of acicular ferrite after thermal treatment. The results confirm that the inclusion chemistry, as affected by the applied deoxidation and desulphurization practice, plays an important role in the microstructure development.

2:50 PM
Graphitisation of Medium-Carbon Steel: Matthew J.W. Green[2]; Philip E. Reynolds[2]; Kejian He[1]; *David V. Edmonds*[1]; [1]University of Leeds, Inst. for Matls. Rsch., Sch. of Process, Environ. & Matls. Engrg., Leeds, W. Yorkshire LS2 9JT UK; [2]Corus Research, Dvlp. & Tech., Swinden Tech. Ctr., Rotherham, S. Yorkshire S60 3AR UK

The effects of different starting microstructures; martensite, bainite and pearlite on the graphitisation processes occurring during graphitisation annealing at 680¨¬C of an experimental 0.39wt% carbon steel, alloyed to accelerate graphitisation times, have been studied using light and transmission electron microscopy. It has been found that the graphitisation process depends upon the starting microstructure; martensite and bainite giving relatively rapid graphitisation rates with pearlite taking approximately an order of magnitude longer. Moreover, much more densely distributed graphite nodules, with a diameter ~3¥ìm, were produced from bainite compared with ~5¥ìm for fine martensite. In contrast, a pearlitic starting microstructure produced much larger nodules, ~34¥ìm in diameter, and with a correspondingly lower nodule count per unit area. This behaviour is considered in terms of the characteristics of the different starting microstructures controlling the dissolution of the cementite phase and nucleation of the graphite phase.

3:15 PM Break

3:25 PM
Heterogeneous Nucleation in HSLA and Electrical Steels: *Kenneth Calvin Russell*[1]; [1]Massachusetts Institute of Technology, Matls. Sci. & Engrg., Rm. 13-5050, 77 Mass. Ave., Cambridge, MA 02139-4307 USA

Classical nucleation theory considers interfaces in solids as two-dimensional continua. Precipitate nucleation is as likely at one location as another and all precipitates are predicted to have the same orientation relationship with the adjacent grains. Modern Coincident Site Lattice (CSL) theory depicts interfaces as complex grids of dislocations that are far removed from two-dimensional continua. Both catalytic potency and precipitate orientation will vary from point to point. Production of quality HSLA and electrical steels requires interfacial precipitates with the correct location and orientation. This paper outlines the considerations the theory for nucleation on the CSL interfaces in these two steel classes and makes recommendations for optimization of properties.

3:50 PM
In-Situ Determination of the Ferrite Nucleation and Growth Rates and its Relation to the Austenite Grain Size Distribution: *Sven Erik Offerman*[1]; Niels van Dijk[2]; Jilt Sietsma[1]; Erik Mejdal Lauridsen[3]; Larry Margulies[3]; Stephan Grigull[4]; Henning Friis Poulsen[3]; Sybrand van der Zwaag[5]; [1]Delft University of Technology, Matls. Sci. & Engrg., Rotterdamseweg 137, Delft 2628 AL The Netherlands; [2]Delft University of Technology, Interfaculty Reactor Inst., Mekelweg 15, Delft 2629JB The Netherlands; [3]Risø National Laboratory, Ctr. for Fundamental Rsch.; Metal Struct. in 4D, Frederiksborgvej 399, PO 49, Roskilde DK-4000 Denmark; [4]European Synchrotron Radiation Facility, BP 220, Grenoble 38043 France; [5]Delft University of Technology, Aeros. Engrg., Kluijverweg 1, Delft 2629 HS The Netherlands

Understanding the grain nucleation and growth mechanisms during solid-state phase transformations requires insight into the relation between the newly formed phase and the parent microstructure. Experiments with the three-dimensional x-ray diffraction (3DXRD) microscope at the European Synchrotron Radiation Facility (ESRF) have been performed to determine in one single measurement the nucleation and growth rates of individual ferrite grains and the austenite grain size distribution before the isothermal transformation in medium carbon steel. This gives information about the relation between the ferrite and austenite microstructures. The in-situ measurements show that the balance between the ferrite nucleation and growth rates changes as a function of undercooling. Lowering the temperature after the first annealing step shows that few new ferrite nuclei form and that the transformation mainly proceeds by the growth of existing ferrite grains. Based on the experimental results a model is presented for the evolution of the microstructure as a function of undercooling.

Product Application and Development: Session II

Sponsored by: AIST, AIST - Division VI
Program Organizers: E. Buddy Damm, The Timken Company, Canton, OH 44706-0930 USA; Amy Bailey, TXI - Chaparral Steel, Midlothian, TX 76065 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Monday PM — Room: La Galerie 5
September 27, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Per Munter, Hatch Associates Ltd., Mississagua, ON L5K2R7 Canada; Pete Jarocewicz, The Timken Company, Appln. Devpt. & Tech. Serv., Canton, OH 44706-0930 USA

2:00 PM
Ultrahigh Magnetic Field (UHMF) Processing: Altering Phase Transformation Kinetics and Microstructural Evolution in Several Ferromagnetic Materials: *R. A. Jaramillo*[1]; G. M. Ludtka[1]; R. A. Kisner[2]; D. M. Nicholson[3]; J. B. Wilgen[2]; G. Mackiewicz-Ludtka[1]; P. N. Kalu[4]; [1]Oak Ridge National Laboratory, Metals & Ceram., Oak Ridge, TN 37831 USA; [2]Oak Ridge National Laboratory, Engrg. Sci. & Tech., Oak Ridge, TN 37831

USA; [3]Oak Ridge National Laboratory, Computer Sci. & Math., Oak Ridge, TN 37831 USA; [4]FAMU-FSU, Coll. of Engrg. & Natl. High Magnetic Field Lab., Tallahassee, FL 32310 USA

Current research Oak Ridge National Laboratory is validating the premise that UHMF processing of ferromagnetic materials can significantly alter phase transformation kinetics and microstructural evolution. This presentation will discuss results and ramifications from some experiments performed using a 33T maximum field strength magnet at the National High Magnetic Field Laboratory. For these experiments, a Fe-15Ni binary, a SAE 1045 and a 52100 steel were exposed to various thermal histories both with and without a magnetic field. Temperature measurements, metallography and hardness measurements indicate a significant shift in phase transformation kinetics and resulting microstructure. Temperature data shows that the transformation temperature during continuous cooling is increased by as much as 90°C in the presence of a 30T magnetic field. These results are supplemented by the resulting microstructures that reveal a significant modification in product phase volume fractions.

2:25 PM
Environment Degradation of Martensitic Stainless Steels for Transmutation Applications: Ajit K. Roy[1]; *Phani P. Gudipati*[1]; Venkataramakrishnan Selvaraj[1]; [1]University of Nevada, Mechl. Engrg., 4505 S. Maryland Pkwy., Las Vegas, NV 89154 USA

Efforts are ongoing to select numerous viable options to dispose high-level nuclear waste. In addition to the proposed geologic disposal of the spent nuclear fuel (SNF) with long half-lives, an alternate method known as transmutation is being considered to reduce their radioactivity. Transmutation refers to the minimization or elimination of long lived actinides and fission products from these SNF by bombarding proton-induced-neutrons onto them. These neutrons are produced by impinging accelerated-driven protons onto a target such as molten Lead-Bismuth-Eutectic (LBE) that will be contained inside a structural sub-system made of martensitic alloys (Alloys EP-823 and HT-9). During the transmutation process, these martensitic alloys may undergo environment induced degradation such as stress corrosion cracking (SCC), hydrogen embrittlement and localized corrosion. In view of this rationale, tests are ongoing involving both alloys in molten LBE and aqueous solutions of different pH values using different state-of-the-art testing techniques. This paper will present the results of SCC and localized corrosion (pitting and crevice) studies. Further, the results of metallographic and fractographic evaluations using optical microscopy and scanning electron microscopy respectively, will be presented.

2:50 PM
Theoretical Substantiation and Commercial Application of a New Plug Tube Drawing Method: *Craig V. Darragh*[1]; [1]The Timken Company, Tech./ Matls. Tech., PO Box 6930, Canton, OH 44706-0930 USA

The conventional method of cold plug drawing of tubes provides for a rigid connection of the drawing plug with its rod (i.e., without transverse displacement relative to each other). Based on the results of theoretical investigations, a new design of the plug assembly has been proposed. In this case, the position of the plug at the stationary stage of the drawing process is defined by equilibrium of the plug alone under the influence of the forces acting on it in the deformation zone. Testing of the plug assembly of the proposed design in drawing 92.0 x 6.0mm tubes has shown the feasibility of making tubes with cross-sectional wall thickness variation of +/-0.6%S and diameter tolerance of +0.15%D.

3:15 PM
The Effect of Boron on Low Carbon Rods and Galvanised Wires: *A. Brownrigg*[1]; A. Wallace[2]; L. Frawley[2]; P. D. Hodgson[1]; [1]Deakin University, 221 Burwood Hwy., Burwood, Victoria 3125 Australia; [2]Smorgon Steel

One of the major factors affecting the quality of EAF steels is high levels of residual nitrogen in the finished product. Nitrogen in interstitial solid solution can increase the risk of failure for applications where a high ductility is required. A simple yet effective way of controlling this problem is by adding nitride-forming elements to the molten steel so that the nitrogen is removed from solution. This paper examines the effect of adding boron to low carbon steels that are used for high formability galvanised wire applications and where the expected benefit is a reduction in yield and tensile strength and an improvement in ductility. 0.06%C and 0.15%C steels were rolled to 5.5mm dia rod and then cold drawn to 2.5mm wire. At this stage the wires were annealed, pickled and then galvanised. When the properties of plain carbon and boron steels were compared it was found that boron caused a significant reduction in work hardening during wire drawing and an improvement in the ductility of the galvanised wire, as measured by torsion testing. The paper will present property and microstructural comparisons from all stages of the steel processing.

3:40 PM Break

4:00 PM
Optimization of Distortion and Mechanical Properties in a Line Pipe Steel: Brian Wolf[1]; *Prabir K. Chaudhury*[1]; [1]General Dynamics, 1200 N. Glenbrook Dr., Garland TX 75046 USA

Heat treatment of a line pipe steel was investigated to determine the optimum processing conditions for adequate mechanical properties and minimum distortion during quenching of steel. Bars of line pipe steel was machined from the pipe stock and heat treated to obtain a minimum yield strength of 70 ksi, ultimate tensile strength of 105 ksi, and elongation of 16%. Hardening treatment was conducted with a wide range of quench rates by varying the austenitizing and quenching temperatures. The distortion and mechanical properties were measured after tempering the steel. Microhardness tests were conducted to determine the depth of hardening. The results show that the amount of martensitic transformation has a strong influence on mechanical properties as well as distortion. The results of this investigation will be presented in the light of optimization of heat treatment process for distortion control in low hardenability steels.

4:25 PM
Development of an Austenitic Structural Steel: *Susil K. Putatunda*[1]; [1]Wayne State University, Matls. Sci. & Engrg., 5050 Anthony Wayne Dr., Rm. 1135, Detroit, MI 48202 USA

In this investigation a new low alloy austenitic structural steel has been developed. This steel after melting and casting and hot rolling has a pearlitic microstructure which can be spherodize annealed to attain good machinability. After austenitizing at 1150°C (2100°F) and water quenching, it has a fully austenitic (100%) microstructure. Because of the fully austenitic structure, it is non-ferromagnetic and has many of the other advantages of austenitic steels i.e., high work hardening rate, good creep resistance and high strength and ductility. A major application of this steel is expected to be in power generation devices such as turbines, generators etc. There will be very little power loss in power generation devices due to low permeability and the non-magnetic nature of austenite.

4:50 PM
Influence of a Novel Two-Step Austempering Process on the Strain Hardening Behavior of Austempered Ductile Cast Iron (ADI): *Susil K. Putatunda*[1]; [1]Wayne State University, Matls. Sci. & Engrg., 5050 Anthony Wayne Dr., Rm. 1135, Detroit, MI 48202 USA

An investigation was carried out to examine the influence of a novel two-step austempering process on the strain hardening behavior of austempered ductile cast iron (ADI). Two batches of cylindrical tensile specimens were prepared from nodular ductile cast iron and austempered by the conventional single-step austempering process and by a novel two-step austempering process. Strain hardening exponent (n value) of all these specimens were determined over the entire plastic deformation regions of the stress-strain curves. Optical microscopy and X-ray diffraction analysis were performed to examine mechanisms of strain hardening behavior in ADI under monotonic (tensile) loading. Test results show that this novel two-step process has resulted in finer ferrite and austenite, higher volume fraction of austenite and higher austenitic carbon. Two-step process has resulted in lower strain hardening exponent compare to conventional austempering process. There also exist a critical austempering temperature below which strain hardening exponent decreases with increase in temperature and above which the strain hardening exponent increases with increase in austempering temperature.

5:15 PM
Microstructure Evolution of a Medium-Carbon Steel During Equal Channel Angular Pressing: *Jingtao Wang*[1]; Guanghai Feng[2]; Du Znongze[2]; Zheng Zhang[2]; Xicheng Zhao[2]; [1]Nanjing University of Science and Technology, Dept. of Matls. Sci. & Engrg., Xiaolingwei No. 200, Nanjing, Jiangsu 210094 China; [2]Xi'an University of Architecture & Technology, Sch. of Metallurgl. Engrg., Yanta Rd. 13., Xi'an, Shannxi 710055 China

Equal channel angular pressing (ECAP) was successfully applied on a medium-carbon steel at 500°C via route C up to 4 passes. Microstructure evolution in the ferrite and pearlite during ECAP was investigated by optical and transmission electron microscopy. The initially equiaxed pearlite nodule was sheared to elongated shape in odds ECAP passes, which was restored to equiaxed shape in even passes. After 4 passes of ECAP via route C, the lamellae pearlite nodules evolved into regions of ultrafine-grained ferrite with fine cement particle dispersions, and these regions distributed uniformly in a pre-eutectoid matrix of ultrafine-grained ferrite with a grain size of ~0.4 micrometer. Strain accommodation of the lamellae structure in the initially pearlite nodule is also investigated.

Roll Technology: Cold and Hot Mill Rolls

Sponsored by: AIST, AIST - Division V
Program Organizers: Ron Webber, Dofasco Inc., Hamilton, Ontario L9G 4T1 Canada; Phil Perry, NSC/PMD Nippon Steel, Plant & Machinery Division, Crown Point, IN 46307 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Monday PM Room: La Galerie 1
September 27, 2004 Location: Marriott New Orleans Hotel

Session Chairs: Mike Olson, California Steel Industries, Fontana, CA 92335 USA; Kalyan K. Khan, USS, Techl. Ctr., Monroeville, PA 15146 USA

2:00 PM
Back-Up Roll Chamfer Design, Profile, and Maintenance: *Florent Decultieux*[1]; Michael S. Hoffman[2]; Thomas P. Adams[3]; [1]Akers Sweden AB, Rsch., 640 60, Akers Styckebruk Sweden; [2]Akers National Roll Company, Sales, 1165 Seminole Dr., Crown Point, IN 46307 USA; [3]Akers National Roll Company, Metall., 400 Railroad Ave., Avonmore, PA 15618 USA

Changes in roll geometries and rolling programs to meet demands of strip quality may lead to tougher rolling conditions and more severe loading of rolls. The design and maintenance of back-up roll chamfers and profile have a significant influence upon the stress distribution and concentration within the rolls during rolling, along with the wear conditions of both back-up and work rolls. Optimization of back-up roll chamfers and profile to specific rolling conditions has been developed. Roll shop machining capabilities accompanied with operator training are considered for maintaining the desired practices.

2:25 PM
Forged Semi-HSS Grade for Work Rolls Dedicated to Cold Rolling of Silicon Steel: *Claude Gaspard*[1]; John Ballani[2]; Pierre Thonus[1]; Catherine Vergne[1]; Daniel Batazzi[1]; [1]Akers France and Belgium, Rue de la Barriere, 40, Seraing BE 4100 Belgium; [2]Akers National Roll

Work rolls have undergone numerous developments over the course of the last few years. The first objective was to produce rolls with a greater hardness penetration depth. The grades developed, which contain 3 to 5% chromium, also have better roughness retention. Then resistance to rolling incidents was improved by the grades with a higher tempering temperature. The most recent developments for cold work rolls are focussed on the family of semi-HSS grades. The semi-HSS grades have already proved that they bring about a significant improvement in roll performance. This is the result of both their excellent resistance against rolling incident, and their ability to maintain the roughness during the rolling process. The increase in campaign time results in an increase in productivity of the mill and simplification of the management of the stock of rolls. These indisputable advantages explain why these grades are being used as work rolls for applications that involve tough rolling conditions as silicon steel.

2:50 PM
Use of HSS Rolls to Skip the Chrome Plating in Cold Rolling Applications: *Claude Gaspard*[1]; John Ballani[2]; Pierre Thonus[1]; Catherine Vergne[1]; Daniel Batazzi[1]; [1]Akers France and Belgium, Rue de la Barriere, 40, Seraing BE 4100 Belgium; [2]Akers National Roll

Recent developments for cold work rolls focus on HSS grades, combining good resistance to rolling incident and exceptional roughness retention, permitting chrome plating to be skipped. Due to the particular metallurgy of such grades, adjustments of grinding are necessary. The choice of grinding wheels and parameters have been studied to reach the required quality on roll and rolled sheet surfaces.

3:15 PM Break

3:30 PM
The Properties and Usage Research of Integrated Enhanced ICDP Work Rolls Made by Local Roll Maker for Hot Rolling: *Peng Hui*[1]; Fei Yi Ruo[1]; [1]Baosteel, Admin. Ctr., Fujin Rd., Baoshan, Shanghai 201900 China

A comparison of microstructures of different ICDP and Enhanced ICDP rolls has been made. Additions of the lanthanide series elements and special carbide forms have been studied. An analysis of the oxidation film on the roll surface has been performed. The performance and accident resistance has been compared to other roll grades.

3:55 PM
Five FAQs about Hot Strip Mill Work Rolls: *Karl Heinrich Schroeder*[1]; [1]BRC, British Rollmakers (China) Ltd., Ste. 1401,14/F.Lippo Sun Plaza, 28 Canton Rd., Kowloon, Hong Kong China

Mill experience generates information about roll performance and behavior. Computer simulations calculate temperature development on and below the roll surface under normal rolling conditions. Finite Element calculations reveal the real stresses in a roll. On the base of this information, general answers are given for frequently asked questions concerning wear, oxide layers, sticking, fire-cracks and friction. Some conlusions are completely different from traditional theories and explanations.

4:20 PM
New Roll Technologies and Roll Design Improvements in Tata Steel: *Umesh Singhal*[1]; [1]Tata Steel, Roll Tech. Office, Tisco MB No W201, Tisco Works, Jamshedpur 831001 India

Roll Consumption at Tata Steel has been reduced over the years in both the Flat and Long Product Mills thru: 1) Use of new and better roll materials; 2) Increase in starting diameters of rolls; 3) Salvaging of rolls; 4) Roll design improvements for avoidance of roll failures; and 5) Improvements in Roll Shop practices.

4:45 PM
History of High Speed Steel Rolls in Japan: *Joseph P. Zuccarelli*[1]; Hiroaki Sorano[1]; [1]Hitachi Metals America, Ltd., 222 N. Park Dr., Ste. #2, Kittanning, PA 16201 USA

Our paper will show: 1. Changes in Work Roll Materials in HSM; 2. Improved Performance with HSS; 3. Improvements of Materials and Operating Conditions; 4. Material Development by Manufacturing Methods; 5. Benefits of HSS Rolls; and 6. Future Developments for HSS Rolls.

Selections From International Conference on Advanced High Strength Sheet Steels for Automotive Applications

Sponsored by: AIST
Program Organizer: Roger Pradhan, International Steel Group, ISG Bethlehem Research, Bethlehem, PA 18015-4731 USA; John G. Speer, Colorado School of Mines, Metallurgical and Materials Engineering, Golden, CO 80401 USA

Monday PM Room: Grand Ballroom J
September 27, 2004 Location: Marriott New Orleans Hotel

Program To Be Announced

The Accelerated Implementation of Materials & Processes: Mechanical Properties - Titanium

Sponsored by: TMS - Structural Materials Division, TMS - ASM/MSCTS-Thermodynamics & Phase Equilibria Committee, TMS - EMPMD/SMD-Chemistry & Physics of Materials Committee, TMS - MPMD-Computational Materials Science & Engineering-(Jt. ASM-MSCTS)
Program Organizers: Rollie E. Dutton, Air Force Research Laboratory, AFRL/MLLMP, WPAFB, OH 45433 USA; John E. Allison, Ford Motor Company, Materials Science and Advanced Engineering, Dearborn, MI 48124-2053 USA; John J. Schirra, Pratt & Whitney, East Hartford, CT 06108 USA; Axel van de Walle, Northwestern University, Materials Science and Engineering, Evanston, IL 60208-3108 USA

Monday PM Room: Mardi Gras Ballroom H
September 27, 2004 Location: Marriott New Orleans Hotel

Session Chair: Dennis M. Dimiduk, Air Force Research Laboratory, AFRL/MLLM, Wright-Patterson AFB, OH 45433-7817 USA

2:00 PM
A Combinatorial Approach to the Development of Neural Networks for the Prediction of Composition/Microstructure/Property Relationships in Alpha/Beta Ti Alloys: *Peter C. Collins*[1]; Rajarshi Banerjee[1]; Hamish Fraser[1]; [1]Ohio State University, Matls. Sci. & Engrg., 477 Watts Hall, 2041 College Rd., Columbus, OH 43210 USA

One approach to the provision of a predictive tool capable of predicting property-microstructure-composition relationships for alpha/beta Ti alloys is to use rules-based models, such as neural-networks, which rely on extensive databases. These required databases, relating microstructure to mechanical properties, are not readily available from industry. Consequently, such databases must be generated in a rapid manner. This paper describes the application of a new combinatorial technique for alloy development and database population based on deposition of graded compositions by laser deposition of a blend of elemental powders. Using this technique, alloy variations of Ti-xAl-yV, where $5<x<7$ and $3<y<5$ (all compositions in wt.%) have been produced using the LENS™ process. The samples have been upset, and iso-compositional tensile coupons have been cut. These have been heat-treated to produce a wide variation of microstructural features, and subsequently tested in an Electro-thermal Mechanical Test system. Rigorous stereological procedures have been employed to determine quantitatively the microstructural features, and these together with the alloy and phase compositions have been included in neural networks. The capabilities of these networks in predicting alloy properties, optimizing compositions and determining functional dependencies of properties on microstructural features will be demonstrated. This research has been supported by the US AFOSR, Dr. Craig Hartley as Program Manager.

2:25 PM

Rapid Assessment of Strengths for Gamma Alloy Sheet by Micro-Hardness Measurements: *Young-Won Kim*[1]; Dennis M. Dimiduk[2]; [1]UES, Inc., 4401 Dayton-Xenia Rd., Dayton, OH 45432 USA; [2]Air Force Research Laboratory, Matls. & Mfg. Direct., AFRL/MLLM, Wright-Patterson AFB, OH 45433 USA

This presentation discusses micro-hardness measurements as a tool to assess the tensile strengths of TiAl alloys. Over the years, we have accumulated data sets for various gamma alloy compositions of Rockwell C hardness (RcH) values, measured principally for fully lamellar microstructures, and their corresponding strengths. Statistical analyses have indicated that the RcH values show definite relationships with either yield strength or ultimate tensile strength depending on the strength level. The relationships have been useful in predicting the tensile strengths simply by measuring RcH values on small coupon samples. The relationships, however, are not yet validated on thin-section material such as gamma annealing alloy sheet (<1.1mm). Gamma alloys in sheet form are produced by pack-rolling and stress-relief annealing (normally at 1000°C for 2h). Our recent experiments indicate that sheet material is still thermally unstable even after the treatment and that various annealing treatments may beneficially alter the sheet properties. This implies that current sheet materials are far from being optimized or that application-specific cases require a great deal of optimization efforts. This optimization will need number of strength tests, especially when new alloy systems are explored for sheet processing and applications. Ongoing efforts show that hardness values (both Rockwell and Vickers) can be interrelated to predict the strength levels of thin sheet material. This presentation will evaluate the interrelationships between both macro- and micro-hardness values and alloy strengths, and discuss the use of these relationships to shorten the optimization process for emerging gamma alloy sheet products.

2:50 PM

Linking Microstructural Features to Mechanical Properties in Ti Alloys Using Advanced Stereology Procedures and Computational Tools: *Jaimie S. Tiley*[1]; [1]United States Air Force, AFRL/MLLM, Bldg. 655, WPAFB, OH 45433 USA

Mechanical properties of titanium alloys are driven by microstructural features. Although rapid advances in microscopy allow imaging of these features, the complexity of possible microstructures make it difficult to accurately predict the mechanical behavior of titanium alloys. This research documents the development of stereology and 3-D serial sectioning procedures to capture and characterize features in Ti-6Al-4V, Ti-555, and Ti-550 alloys. This involves various microstructures provided by different processing conditions. In addition, the features are also linked to mechanical properties using advanced neural network and fuzzy logic modeling to provide predictive capabilities and identify important parameters. Samples from each of the alloys and processing conditions were mechanically tested to determine yield strength and ultimate strength at room temperature. Results indicate the through thickness changes in microstructure and importance of lath structures and colony intersections on tensile properties.

3:15 PM

Modeling of Tensile Property - Microstructure Relationships in Timetal 550: *Eunha Lee*[1]; Thomas Searles[1]; Sujoy Kar[1]; Gopal Viswanathan[1]; Rajarshi Banerjee[1]; Hamish Fraser[1]; [1]Ohio State University, Matls. Sci. & Engrg., 477 Watts Hall, 2041 College Rd., Columbus, OH 43210 USA

One of the important requirements for the accelerated insertion of materials in components is the development of tools for predicting property-microstructure relationships in relevant alloys via a synergistic coupling of computational models with critical experimentation. This paper will discuss the development of Fuzzy Logic and Neural Network Models based on Bayesian statistics to predict the yield strength, ultimate tensile strength and elongation of the alpha/beta Ti alloy, Timetal-550, at room temperature. Ti-550 was heat-treated using the Gleeble thermal-mechanical simulator where holding time, cooling rate from high temperatures and heat treatment temperatures were varied to obtain various microstructures. Subsequently, for each heat-treated condition, different microstructural features, spanning across different length scales, were quantified using stereological procedures. The database consisting of these quantified microstructural features together with the corresponding tensile properties has been used to train and test Fuzzy Logic and Neural Network models. These predictive models for tensile properties will be presented. In addition, the use of virtual experiments to predict the functional dependencies of microstructural features on tensile properties will be discussed.

3:40 PM

Neural Network Modeling of Fracture Toughness and Tensile Properties of Alpha/Beta Titanium Alloys Based on Microstructural Features: *Sujoy Kar*[1]; Thomas Searles[1]; Eunha Lee[1]; Jaimie Tiley[1]; Gopal Viswanathan[1]; Rajarshi Banerjee[1]; Hamish Fraser[1]; [1]Ohio State University, Matls. Sci. & Engrg., 477 Watts Hall, 2041 College Rd., Columbus, OH 43210 USA

The development of a set of computational tools that permit microstructurally-based predictions for the fracture toughness and tensile properties of commercially important titanium alloys, such as Ti-6Al-4V, is a valuable step towards the accelerated maturation of materials. This paper will discuss the development of Neural Network Models based on Bayesian statistics to predict the fracture toughness, yield strength, ultimate tensile strength and elongation of Ti-6Al-4V at room temperature. The development of such rules-based models requires the building up of extensive databases, which in the present case are microstructurally-based. The steps involved in database development include controlled variations of the microstructure using thermo-mechanical treatments, the use of standardized stereology protocols to rapidly characterize and quantify microstructural features, and mechanical testing of the heat-treated specimens. These databases have been used to train and test the Neural Network to predict the fracture toughness and tensile properties. In addition, these models have been successfully used to identify the functional dependence of mechanical properties on individual microstructural features via virtual experiments, consequently guiding the efforts towards development of more robust phenomenological models.

Third International Symposium on Railroad Tank Cars: Session II

Sponsored by: AIST, AIST - Division VI
Program Organizers: Murali Manohar, ISG; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Monday PM — Room: Mardi Gras Ballroom B
September 27, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Geoff Dahlman, Burlington Northern Santa Fe Railway, Topeka, KS 66612 USA; Murali Manohar, International Steel Group Research, Bethlehem, PA 18015-4731 USA

2:00 PM

Vertical Coupler Load Environment: *Vinaya Sharma*[1]; [1]Sharma & Associates, Inc., 5810 S. Grant St., Hinsdale, IL 60521 USA

Revenue service tests of tank cars have recorded unexpectedly high coupler vertical forces as part of the service spectrum. Most tank car designs are vulnerable under high coupler vertical forces. To improve the safety of tank car designs and operations, it is necessary to better understand the causes and effects of these forces. A full scale tank car was instrumented, loaded, and tested in static and impact conditions. Significant vertical forces were generated during impact, even in the absence of any coupler height mismatch between impacting cars. It was noted that vertical forces induce 50% of the maximum stress seen at the tank head. Therefore, ignoring the effects of vertical forces will lead to an underestimation of stress levels and fatigue levels in tank cars. Coupler height mismatch further adds to the vertical forces and stresses in critical areas of the stub sill-tank car interface. Stresses were 50% higher when there was a 2" height mismatch. Therefore, it is prudent to minimize coupler height mismatch whenever and wherever practical. The Federal Railroad Administration's (FRA) Office of Research and Development funded this research project.

2:30 PM

Thermographic Inspection and Assessment of Defects in Tank-Car Thermal Protection Systems: *A. Michael Birk*[1]; [1]Queen's University, Dept. of Mechl. & Matls. Engrg., Kingston, Ontario K7L 3N6 Canada

Some rail tank cars are equipped with thermal protection systems for fire protection. One example of this system consists of a 13 mm blanket of ceramic fibre insulation covered by a 3 mm steel jacket. Many of these systems have been in operation for more than 20 years and some have degraded due to tearing and slippage of the insulation. This paper describes the development of a thermographic inspection method for determining if thermal protection defects are present. Some limited field data is also presented which shows that some of the older installations are severely defective. The paper also describes a computer based method for assessing the signficance of the insulation defects.

3:00 PM Break

3:15 PM

Tank Car Steel Investigations: *Roger D. Sims*[1]; [1]Sims Professional Engineers, 2645 Ridge Rd., Highland, IN 46322 USA

Previous studies have shown alternative steels may improve the performance of tank cars when they are involved in railroad accidents. ASTM A841 - Grade C Class 2 microalloyed steel was selected as a candidate for replacing TC-128B steel that is currently used in the manufacturing of tank car heads and shells. A first step in evaluating the manufacturability of tank cars using this new steel was to check its head forming capabilities. The materials sensitivity to heating was evaluated and a limit of 1300°F was established. Warm and cold head forming produced a physically acceptable product but metallurgical problems were discovered. Segregated bands with martinsite streaks produced erratic energy absorption as determined through Charpy tests. Segregation and property variation must be improved in the as-rolled condition before further consideration can be given ASTM A841 - Grade C Class 2 material. Other materials or strategies may be exercised as well.

3:45 PM

Development of a Low Carbon HSLA Alternative to TC128 for Tank Car Application: *D. Bai*[1]; J. Dorricott[2]; F. Hamad[1]; S. Hansen[2]; [1]IPSCO Inc., R&D, 1770 Bill Sharp Blvd., Muscatine, IA 52761 USA; [2]Mobile Works, 12400 Highway 43N, Axis, AL 36505 USA

Traditionally, a medium-carbon steel (produced to the requirements of TC-128) has been the material of choice for tank car fabrication. Consequently, normalizing is required to produce adequate toughness levels when this grade is used in low-temperature service. In contrast, low-carbon, high-strength low-alloy (HSLA) steels develop excellent combinations of strength, toughness and weldability in the as-rolled condition. Based on years of experience with microalloying and thermo-mechanical controlled processing in the production of X70/X80 linepipe steels, IPSCO has developed an HSLA alternative for potential use in tank cars. Important properties of this new grade are presented and compared to characteristics of the current normalized product.

4:15 PM

High-Strength, Low-Carbon, Ferritic, Copper-Precipitation-Strengthening Steels: *Semyon Vaynman*[1]; Morris E. Fine[1]; Shrikant B. Bhat[2]; [1]Northwestern University, Dept. of Matls. Sci. & Engrg., 2225 N. Campus Dr., Evanston, IL 60208 USA; [2]Ispat Inland Inc., Product Applications R&D, 3001 E. Columbus Dr., E. Chicago, IN 46312 USA

Development of higher strength-higher toughness steels for tank car applications has been a target for many years to improve the overall performance of railroad tank cars. Over the past ten years, three grades of low carbon copper-precipitation-hardened steels have been investigated (NUCu-60, NUCu-70 and NUCu-100) in collaborative research between Northwestern University and Ispat-Inland Inc. The two lower-strength grades are produced by air cooling after hot rolling. The NUCu-60 Grade (Supertough Cryogenic Steel) has yield stress of 415 MPa (60 Ksi) and remarkable toughness at cryogenic temperatures; more than 350 J (264 ft-lbs) down to -79C (-110F). The NUCu-70 Grade has at least 485 MPa (70 Ksi) yield strength. Composition of NUCu-100 Grade is the same as that of NUCu-70. The higher strength is achieved by quenching from the austenitizing temperature and aging. The mechanical properties as well as the corrosion resistance and welding properties of these steels will be discussed.

Titanium for Healthcare, Biomedical, and Dental Applications: Beta Titanium Alloys

Sponsored by: TMS - Structural Materials Division, Japan Institute of Metals, TMS - SMD-Titanium Committee, TMS - SMD-Corrosion and Environmental Effects Committee-(Jt. ASM-MSCTS)

Program Organizers: Carl Boehlert, Alfred University, School of Ceramic Engineering and Materials Science, Alfred, NY 14802 USA; Dhanesh Chandra, University of Nevada, Metallurgical and Materials Engineering, Reno, NV 89557 USA; Masahiko Ikeda, Kansai University, Department of Materials Science and Engineering, Suita, Osaka 564-8680 Japan; Mitsuo Niinomi, Toyohashi University of Technology, Department of Production Systems Engineering, Toyohashi 441-8580 Japan

Monday PM — Room: Mardi Gras Ballroom D
September 27, 2004 — Location: Marriott New Orleans Hotel

Session Chair: Mitsuo Niinomi, Toyohashi University of Technology, Dept. of Production Sys. Engrg., Toyohashi 441-8580 Japan

2:00 PM Invited

Mechanical Properties and Cyto-Toxicity of Newly Designed Beta Type Titanium Alloys with Low Melting Points for Dental Applications: *Mitsuo Niinomi*[1]; Toshikazu Akahori[1]; Tsutomu Takeuchi[2]; Shigeki Katsura[3]; Hisao Fukui[4]; [1]Toyohashi University of Technology, Dept. of Production Sys. Engrg., 1-1, Hibarigaoka, Tempak-cho, Toyohashi, Aichi 441-8580 Japan; [2]Takauchikatan Ltd., 203, Motomachi, Minamioshimizu-cho, Toyohashi, Aichi 441-8132 Japan; [3]Yamahachi Dental Co., 54, Ochigara, Nishiura-cho, Gamagori, Aichi 443-0105 Japan; [4]Aichi-Gakuin University, Dept. of Dental Matls. Sci. Sch. of Dentistry, 1-100, Kusumoto-cho, Chikusa-ku, Nagoya, Aichi 464-8650 Japan

Beta type titanium alloy, Ti-29Nb-13Ta-4.6Zr (TNTZ), composed of non-toxic elements with low modulus of elasticity has been developed for biomedical applications. TNTZ expects to be used for dental applications because of excellent mechanical properties and biocompatibility. When TNTZ is applied as dental materials, as-cast products are preferred because complicated shape products are able be obtained by dental precision casting. However, TNTZ has a high melting point and high reactivity with mold. Thus, TNTZ has possibility to have a number of casting defects and thick reaction surface layer associated with mold. They are considered to decrease the mechanical properties of casting products. Ti-Nb-Zr-(Cr, Si and Fe), Ti-Nb-Zr-Cr-Fe and Ti-Nb-Zr-Cr-Si where the highest melting point element, Ta, in TNTZ was replaced with low melting point elements, Cr, Fe, and Si, in order to obtain new beta type titanium alloys with low melting points for dental applications. Their melting points, mechanical properties, microstructures, surface reaction layers and cyto-toxicity were investigated in this study.

2:25 PM

A Novel Combinatorial Approach to the Development of Beta Titanium Alloys for Orthopaedic Implants: *Rajarshi Banerjee*[1]; Soumya Nag[1]; Hamish Fraser[1]; [1]Ohio State University, Matls. Sci. & Engrg., 477 Watts Hall, 2041 College Rd., Columbus, OH 43210 USA

The ideal recipe for a biomaterial to be used for implant applications is excellent biocompatibility with no adverse tissue reactions, excellent corrosion resistance in the body fluid where it will be used, high mechanical strength and fatigue resistance, low modulus, and good wear resistance. Since the beta phase in Ti alloys exhibits a significantly lower modulus than the alpha phase, and the beta alloys also satisfy most of the other requirements for an ideal bioalloy, there is a thrust towards the development lower modulus beta-Ti alloys which retain a single beta phase microstructure on rapidly cooling from high temperatures. Biocompatible beta-Ti alloys, reported in the literature, include Ti-12Mo-6Zr-2Fe (‘TMZF’), Ti-15Mo-5Zr-3Al, Ti-15Mo-3Nb-3O(‘TIMETAL 21Srx’), Ti-14Nb-13Zr, Ti-35Nb-5Ta-7Zr(‘TNZT’), and Ti-15Mo. While these alloy compositions are promising, there is still a tremendous scope for improvement in terms of alloy design via optimization of alloy composition and thermo-mechanical treatments. Rules-based modeling approaches can be a very effective method for such optimization studies. From the available literature reports on beta-Ti alloys, a database relating composition variables to modulus and yield strength to has been compiled. This database has been used to train a Fuzzy-logic model relating the same composition variables to the mechanical properties. The trained model has been used to predict the influence of different alloying additions on the modulus and yield strength and consequently employed to identify optimum alloy compositions in the Ti-Nb-Zr-Ta alloy system. Using laser deposition, compositionally graded alloys have been deposited based on the promising compositions identified based on the modeling efforts. The mechanical properties of these alloys and the influence of thermo-mechanical processing on the properties will be discussed. Initial studies on biocompatibility assessment of these alloys will also be presented. This approach allows for the rapid assessment and screening of promising alloy compositions for implant applications and is expected to be an useful combinatorial tool for the development of new orthopaedic alloys.

2:50 PM
Microstructural Evolution and Strengthening Mechanisms in Ti-Nb-Zr-Ta, Ti-Mo-Zr-Fe and Ti-15Mo Biocompatible Alloys: *Soumya Nag*[1]; Rajarshi Banerjee[1]; Hamish Fraser[1]; [1]Ohio State University, Matls. Sci. & Engrg., 477 Watts Hall, 2041 College Rd., Columbus, OH 43210 USA

The microstuctural evolution and the strengthening mechanisms in the two quaternary alloys, TNZT (Ti-34Nb-9Zr-8Ta) and TMZF (Ti-13Mo-7Zr-3Fe), and one binary alloy, Ti-15Mo, have been investigated. In the homogenized condition both the quaternary alloys exhibited a microstructure consisting primarily of a beta-Ti matrix with grain boundary alpha precipitates and a low volume fraction of primary alpha precipitates while the binary alloy showed single phase microstructure with large beta grains. On ageing the homogenized alloys at 6000C for 4 hours, all the alloys exhibited the precipitation of refined scale secondary alpha precipitates distributed homogeneously in the beta matrix. However, after ageing while the hardness of TMZF marginally increased, that of the TNZT and Ti-15Mo alloys decreased. Furthermore the modulus of TNZT decreased while other two alloys showed opposite trends. To understand these differences in mechanical properties after ageing, TEM studies have been carried out on all the alloys in homogenized and homogenized plus ageing conditions. The results indicate that in TNZT existence of metastable B2 ordering in homogenized condition results in high hardness and modulus values. This chemical ordering is destroyed after ageing and the B2 to beta transformation causes a reduction in both hardness and modulus of this alloy. Also in Ti-15Mo, dissolution of omega precipitates on ageing cause the hardness to reduce, while the precipitation of secondary alpha causes an increase in the modulus. Using these examples the important influence of thermal processing on the property-microstructure relationships in orthopaedic alloys for implant applications will be highlighted.

3:15 PM Break

3:25 PM Invited
The Effect of Aluminum on Phase Constitution and Heat Treatment Behavior in Ti-Cr-Al Alloys for Healthcare Applications: Masahiko Ikeda[1]; *Daisuke Sugano*[2]; [1]Kansai Uinversity, Dept. of Matls. Sci. & Engrg., 3-3-35, Yamate-cho, Suita, Osaka 564-8680 Japan; [2]Kansai University, Grad. Student, 3-3-35, Yamate-cho, Suita, Osaka 564-8680 Japan

Since the life expectancy is increasing, it is very important to develop reliable functional materials for healthcare applications. Though titanium and its alloys are one of the attractive metallic materials for the healthcare application, these alloys are expensive. The present investigation suggests to reduce the cost by using new low cost beta Ti alloys. For reliability, heat treatment behavior of beta Ti alloys, Ti-7mass%Cr, with Al percentage varying from 0, 1.5, 3.0 and 4.5, is investigated using electrical resistivity and Vickers hardness measurements. In Ti-7Cr-0Al alloy quenched from 1173K, only beta phase was identified by X-ray diffraction (XRD). In Ti-7Cr-1.5 to 4.5Al alloys, beta and orthorhombic martensite were identified by XRD. On isochronal heat treatment of Ti-7Cr-3Al and Ti-7Cr-4.5Al, resistivity at liquid nitrogen temperature and resistivity ratio were increased at temperatures between 423K and 523K because of reverse transformation of orthorhombic martensite to metastable beta phase.

3:50 PM
Microstructures and Mechanical Properties of Low Cost Beta-Titanium Alloy for Healthcare Applications: *Guna Warman*[1]; Mitsuo Niinomi[1]; Toshikazu Akahori[1]; Takayuki Souma[1]; Masahiko Ikeda[2]; [1]Toyohashi University of Technology, Dept. of Production Sys. Engrg., 1-1 Hibarigaoka, Tempaku-cho, Toyohashi, Aichi-ken 441-8580 Japan; [2]Kansai University, Dept. of Matls. Sci. & Engrg., 3-3-35 Yamate-cho, Suita, Osaka 564-8680 Japan

Titanium alloys are the best choice of metallic materials for biomedical and healthcare applications due to the combination of its excellent mechanical properties and biocompability. However, the usage of titanium alloys is limited because its high cost. In purpose to reduce the cost, two kind of titanium alloys, Ti-4.3Fe-7.1Cr (TFC) and Ti-4.3Fe-7.1Cr-3.0Al (TFCA), for healthcare goods such as wheelchairs has been recently developed using low cost ferro-chrom elements or recycled titanium containing Fe. This study investigates the microstructure and mechanical properties of the alloys solution treated in beta field. The fatigue ratios of TFC and TFCA alloys are much higher than those of other metallic materials. Uncrystalized grains obtained in the alloys at low solution treatment temperature can be omitted by increasing solution treatment temperature or by conducting thermomechanical treatment. The latter method is recommended because it gives smaller grain size and thus better strength and ductility balance.

4:15 PM
Decomposition of Ti-29Nb-13Ta-4.6Zr Alloy at Intermediate Temperature: Shu Jun Li[1]; *Rui Yang*[1]; Mitsuo Niinomi[2]; Yu Lin Hao[1]; Zheng Xiao Guo[3]; [1]Chinese Academy of Sciences, Inst. of Metal Rsch., Shenyang Natl. Lab. of Matls., 72 Wenhua Rd., Shenyang, Liaoning Province 110016 China; [2]Toyohashi University of Technology, Dept. of Productions Sys. Engrg., 1-1 Hibarigaoka, Tempaku-cho, Toyohashi 441-8580 Japan; [3]Queen Mary, University of London, Dept. of Matls., Mile End Rd., London E1 4NS UK

Ti-29Nb-13Ta-4.6Zr (wt%) is a β type alloy for biomedical applications and has a solution treated microstructure of (β+α”) after ice-water quenching but of (β+ω) after air or furnace cooling. The decomposition of the alloy during aging at intermediate temperatures of 300 to 500°C was found to depend on both temperature and the starting microstructure: The ω phase formed during aging below about 400°C whereas the α formed after aging above 350°C. In the temperature range in which the two phases co-precipitate, a higher volume fraction of ω results for the starting microstructure of (β+ω) but α phase dominate the aged microstructure for the starting microstructure of (β+α”). This difference has been attributed to α” martensite acting as nuclei of the α phase, thus providing a shortcut path to the precipitation of α at the expense of ω.

4:40 PM
Mechanical Properties and Microstructures of New Ti-Fe-Ta and Ti-Fe-Ta-Zr System Alloys: *Daisuke Kuroda*[1]; Hironori Kawasaki[1]; Akiko Yamamoto[1]; Sachiko Hiromoto[1]; Takao Hanawa[1]; [1]National Institute for Materials Science, Biomatls. Ctr., 1-2-1, Sengen, Tsukuba, Ibaraki 305-0047 Japan

Beta-type titanium alloys consisting of non-toxic elements, Ti-8Fe-8Ta, Ti-8Fe-8Ta-4Zr and Ti-10Fe-10Ta-4Zr alloys in mass%, were newly designed and developed for biomedical applications. Changes in the mechanical properties of the alloys with various heat treatments are discussed on the basis of the resultant microstructures. Structural phase of these alloys after cold forging and solution treatment was only beta phase. Ti-8Fe-8Ta and Ti-8Fe-8Ta-4Zr have higher strength than those of conventional biomedical titanium alloys such as Ti-6Al-4V ELI, Ti-6Al-7Nb and Ti-13Nb-13Zr. Corrosion resistance of Ti-8Fe-8Ta and Ti-8Fe-8Ta-4Zr after cold forging and solution treatment was higher than that of cp-Ti and Ti-6Al-4V ELI. Therefore, new beta-type titanium alloys designed in this study, Ti-8Fe-8Ta and Ti-8Fe-8Ta-4Zr, are expected to have good properties as biomaterials.

Use of Bainitic and Bainitic-Martensitic Steels in Current or Developing Applications

Sponsored by: AIST, AIST - Division VI
Program Organizers: Helio Goldenstein, University of San Paulo, Cidade Universitaria, 05508-900 - Sao Paulo Brazil; Dengqi Bai, IPSCO Inc., Muscatine, IA 52761 USA; E. Buddy Damm, The Timken Company, Canton, OH 44706-0930 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Monday PM — Room: Mardi Gras Ballroom C
September 27, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: E. Buddy Damm, The Timken Company, Matls. R&D, Canton, OH 44706 USA; Dengqi Bai, IPSCO Inc., Muscatine, IA USA; Helio Goldenstein, University of San Paulo, Sao Paulo 05508-900 Brazil

2:00 PM
Meeting Specification, Failing Expectations: *Krishnaswamy Sampath*[1]; [1]Consultant, 615 Demuth St., Johnstown, PA 15904 USA

Manufacturers of US Navy submarines and aircraft carriers use heavy-gage (3-inches and over) HY-100 grade steel plates for fabricating certain critical structures that resist shock, blast, and ballistic loading. These steel plates are currently produced to MIL-S-16216K (SH) specification which does not specify required aluminum content. Furthermore, the through-thickness ductility of the rolled plate is an important property for these structures, although achieving a minimum through-thickness ductility is not a requirement in the current MIL-S-16216K (SH) or its predecessor MIL-S-16216J (SH) specification. A 20% minimum reduction in area (%RA) in through-thickness ductility is introduced during plate procurement. Heavy-gage HY-100 plates that meet the specification do not necessarily meet the ductility requirement. Research showed that restoring aluminum and sulfur contents to 1983 First article qualification test practice levels offered the most cost-effective method for achieving the required through-thickness ductility.

2:25 PM
Hyper-Strength Bainitic Steels: *Peter Brown*[1]; [1]QinetiQ, FST/Advd. Metallics Grp., Bldg. A7, Rm. 2008, Ively Rd., Farnborough, Hampshire GU149PW England

The microstructure and mechanical properties of three hyper-strength (HYS) bainitic steels developed using computer-based thermodynamic modelling techniques are discussed. Progressive mechanical property improvements, particularly tensile ductility, achieved with each modelling iteration are highlighted. The exploitation of isothermal hardening, a new strengthening mechanism observed in high carbon, high silicon HYS bainitic steels, is also reported. The use of low-cost HYS bainitic steels for demanding commercial and defence applications is then outlined with special emphasis being placed on significant reduction in product lead times in association with the use of computer-based thermodynamic modelling techniques.

2:50 PM
Effect of Aluminium on Stability of Retained Austenite in Austempered Ductile Irons: *A. R. Kiani-Rashid*[1]; D. V. Edmonds[2]; [1]University of Sistan & Baluchestan, Dept. of Matls., Faculty of Engrg., Zahedan, Sistan & Baluchestan 9816745563-161 Iran; [2]University of Leeds, Leeds UK

The microstructure of ADI consists of nodular graphite that is randomly dispersed in a bainitic matrix consisting of bainitic ferrite and carbon enriched retained austenite. This form of bainite is unique in that it contains little or no carbide, despite the high carbon concentration. The presence of well distributed graphite in the matrix, and a relatively high volume fraction of retained austenite, are responsible for the good mechanical properties of the austempered ductile irons including excellent wear resistance. It is now well known that the notable properties of ADI directly depend on the volume fraction of retained austenite in the matrix. Consequently, the influence of the aluminium on the detailed microstructure of as-cast and heat treated irons and the final properties are examined.

3:15 PM
Microstructure and Hardness of Grade 9260 Steel Heat-Treated by the Quenching and Partitioning (Q&P) Process: *Florian Gerdemann*[1]; John G. Speer[2]; David K. Matlock[2]; [1]RWTH Aachen University, Dept. of Ferrous Metall., Intzestr. 1, Aachen 52072 Germany; [2]Colorado School of Mines, Advd. Steel Procg. & Products Rsch. Ctr., Golden, CO 80401 USA

This paper summarizes the results of a research project examining icrostructure development using the Quenching and Partitioning process on a bar steel grade 9260. In theory the Q&P process can produce a microstructure consisting of carbon depleted martensite, carbon enriched retained austenite and carbon-supersaturated martensite. The aim of this project was to predict the possible microstructure and carbon enrichment using the Q&P process and compare the calculated results with experimental data. Hardness results were also obtained, and correlated with microstructure and processing. Conventional heat treatments including quenching and tempering, and austempering were also conducted for comparison with the results of the Q&P process. The predicted quench temperature for maximum retained austenite closely matched with the experimental data, although the actual austenite levels were somewhat lower than the values hypothesized for ideal carbon partitioning behavior. Some attractive combinations of hardness and retained austenite were identified.

3:40 PM Break

4:00 PM
Atom Probe Analysis of Carbon Distribution in a Bainitic High-Strength Steel: Mathew Peet[2]; *Sudarsanam S. Babu*[1]; Michael K. Miller[1]; H. K.D. H. Bhadeshia[2]; [1]Oak Ridge National Laboratory, Metals & Ceram. Div., 1, Bethel Valley Rd., Bldg. 4508, MS 6096, Oak Ridge, TN 37831-6096 USA; [2]University of Cambridge, Dept. of Matls. Sci. & Metall., Pembroke St., Cambridge CB23QZ UK

An energy compensated optical position sensitive atom probe was used to analyze the nanoscale distribution of carbon and other substitutional solutes in a low temperature bainitic microstructure consisting of a mixture of bainitic ferrite plates in a retained austenite matrix. Atom probe microanalysis showed a wide distribution of carbon concentrations in both ferrite and austenite. The ferrite carbon concentrations are higher than the expected paraequilibrium solubility levels and the austenite carbon concentration is found to be slightly higher than the T0 limit. The results are consistent with previous atom-probe data on low carbon steels and confirm X-ray data, which indicated excess carbon in bainitic ferrite. Research at the Oak Ridge National Laboratory SHaRE User Center was sponsored by the Division of Materials Sciences and Engineering, U.S. Department of Energy, under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

4:25 PM
Altering Phase Transformation Kinetics and Microstructural Evolution in High Strength Bainite Steel via Ultrahigh Magnetic Field (UHMF) Processing: *Roger A. Jaramillo*[1]; G. M. Ludtka[1]; S. S. Babu[1]; R. A. Kisner[2]; G. Mackiewicz-Ludtka[1]; [1]Oak Ridge National Laboratory, Metals & Ceram., PO Box 2008, Oak Ridge, TN 37831-6064 USA; [2]Oak Ridge National Laboratory, Engrg. Sci. & Tech., Oak Ridge, TN 37831 USA

Current research Oak Ridge National Laboratory is validating the premise that UHMF processing of ferromagnetic materials can significantly alter phase transformation kinetics and microstructural evolution. This presentation will discuss results and ramifications from some experiments performed using a 33T maximum field strength magnet at the National High Magnetic Field Laboratory. A recently developed high strength bainitic steel was exposed to continuous cooling and an isothermal hold both with and without a 30T magnetic field. Temperature measurements, metallography and hardness measurements indicate a significant shift in phase transformation kinetics and resulting microstructure. The application of a magnetic field during continuous cooling of a high strength bainitic steel has produced a pearlitic microstructure not possible without the additional thermodynamic driving force associated with a 30T magnetic field.

4:50 PM
Comparison of Three Ni-Hard I Alloys: *Omer N. Dogan*[1]; [1]U.S. Department of Energy, Albany Rsch. Ctr., 1450 Queen Ave., SW, Albany, OR 97321 USA

An investigation was undertaken to reveal the similarities and differences in the mechanical properties and microstructural characteristics of three Ni-Hard I alloys with varying alloying elements. These alloyed white cast irons are used primarily in applications requiring superior wear resistance. The alloys were evaluated in both as-cast and stress-relieved conditions. While the matrix of the high Ni alloys is composed of austenite and martensite in both conditions, the matrix of the low Ni alloy consists of a considerable amount of bainite, in addition to the martensite and the retained austenite in as cast condition, and primarily bainite, with some retained austenite, in the stress relieved condition. It was found that the stress relieving treatment does not change the tensile strength of the high Ni alloy. Both the as cast and stress relieved high Ni alloys had a tensile strength of about 350 MPa. On the other hand, the tensile strength of the low Ni alloy increased from 340 MPa to 452 MPa with the stre ss relieving treatment. There was no significant difference in the wear resistance of these alloys in both as-cast and stress-relieved conditions.

5:15 PM
Investigation on a New Type of Bainite Ductile Iron Suitability for Rolling: *Ji Chengchang*[1]; Zhu Shigen[2]; Wu Dehai[3]; [1]Donghua University, Sch. of Mechl. Engrg., 1882 Yan'an Rd. W., Shanghai, 200051 China; [2]Donghua University, Coll. of Matl. Sci. & Engrg., 1882 Yan'an Rd. W., Shanghai, 200051 China; [3]Tsinghua University, Sch. of Mechl. Engrg., Beijing 100084 China

A new type ductile iron suitability for rolling was studied. With a suitable ausforming and special quenching medium, metallurgical structure with acicular structure (bainite and martensite), some austenite and cementite can be obtained. The impact toughness and the hardness is about 30 J/cm2 and HRC55, respectively. Bars with different diameters were prepared by horizontal continuous casting. Experiments of from bar to plate and thin bar were carried out utilizing rolling mill. The results indicate that this material can be rolled and the total cross compress ratio from bar to plate and to thin bar can be up to 70% and 77%, respectively. Grinding balls with Ö35mm to Ö60mm were produced with a skew rolling mill. Ö80mm grinding balls were also produced by die forging. Falling sphere tests indicate that the falling times from 3.5m height is over 40000. and this resistant material will be of a wide uses.

3-Dimensional Materials Science: X-Ray Techniques

Sponsored by: TMS - Structural Materials Division
Program Organizers: Marc J. De Graef, Carnegie Mellon University, Department Material Science & Engineering, Pittsburgh, PA 15213-3890 USA; Jeff P. Simmons, Air Force Research Laboratory, Materials & Manufacturing Directorate, Dayton, OH 45433 USA; George Spanos, Naval Research Laboratory, Physical Metallurgy Branch, Washington, DC 20375-5000 USA; Jonathan E. Spowart, UES Inc., Dayton, OH 45432 USA

Tuesday AM — Room: Mardi Gras Ballroom F/G
September 28, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Jonathan E. Spowart, UES, Inc., Wright-Patterson AFB, OH 45433-7817 USA; Dorte Juul-Jensen, Riso National Laboratory, Ctr. for Fundamental Rsch., Roskilde DK 4000 Denmark

8:30 AM Invited
Non-Destructive 3D Mapping of Grain Structures: *Dorte Juul-Jensen*[1]; [1]Riso National Laboratory, Ctr. for Fundamental Rsch., Metal Struct. in Four Dimensions, Roskilde DK4000 Denmark

This presentation overviews this year's improvements and progress of the 3 Dimensional X-Ray Diffraction (3DXRD) method. The improvements include i) implementation of a new detector which hopefully will lead to a significant improved spatial resolution below the present 5umx5umx1um and ii) introduction of new software for reconstruction of microstructures from the diffraction spots which is more user-friendly and allows faster measurements. Progress is achieved in the full 3D reconstruction of grain structures. Data for pure aluminum are presented. In order to verify the 3DXRD results, a test sample was after the 3DXRD experiments characterized using classical serial sectioning (by polishing) and EBSP to map the structure. The results of the two methods are compared and discussed. Finally in-situ 3DXRD data for the growth of bulk grains during recrystallization are presented and implications for modelling are discussed.

9:00 AM
Liquid Ga Penetration into an Aluminium Alloy by High-Resolution X-Ray CT: *Tomomi Ohgaki*[1]; Hiroyuki Toda[1]; Ian Sinclair[2]; Jean-Yves Buffière[3]; Wolfgang Ludwig[3]; Toshiro Kobayashi[1]; [1]Toyohashi University of Technology, Dept. of Production Sys. Engrg., 1-1 Hibarigaoka, Tempaku-cho, Toyohashi, Aichi 441-8580 Japan; [2]University of Southampton, Matls. Rsch. Grp., Sch. of Engrg. Scis., Highfield, Southampton SO17 1BJ UK; [3]INSA de Lyon, Grp. d'Etudes de Metallurgie Physique et de Physique des Materiaux, Unite Mixte de Recherche associee au CNRS 5510, Lyon, 20 ave. A Einstein, 69621 Villeurbanne, Cedex France

For clear 3D visualization of the grain boundaries and the crack, the penetration of liquid Ga has been performed in an Al alloy. The advance directions of the crack-tip were strongly dependent on the grains and the separation of the crack originates from grain distribution. The 3D expansion of the Al volume, the volume reduction of micropores, and the brittle fracture were evidently observed due to the Ga penetration. The 3D mapping of the pore's displacements in the Al alloy before and after Ga penetration has been obtained and the complicated 3D distribution of strains between the grains were grasped in micron level by microstructural gauging technique which is the utilization of the micropores as marker points and the Ga penetration. In this study, we have acquired the fundamental information for the microstructural gauging technique by Ga penetration.

9:20 AM
Understanding the Rapid Solidification of Al-5Cu and Al-17Cu Using X-Ray Tomography: *Arvind Prasad*[1]; Hani Henein[1]; Eric Maire[2]; Charles-Andre Gandin[3]; [1]University of Alberta, Advd. Matls. & Procg. Lab., Dept. of Chem. & Matls. Engrg., Edmonton Canada; [2]INSA, GEMPPM, Lyon, Villeurbanne 69621 France; [3]Ecole des Mines de Nancy, Nancy France

X-Ray tomography using Synchrotron radiation with 1 µm beam resolution at ESRF was used to generate 3D images for rapidly solidified Al 5% and 17% Cu atomized 500 µm droplets. Microstructural features of solidification, such as, nucleation and initial growth, shrinkage etc. that were apparent in the 3D images will be reported. The coordinates of the single nucleation site was evaluated and the weight fraction of initial growth regime of solidification was successfully quantified. This presentation will also report on the quantification of the total recalescence region and the porosity distribution within the droplets. These observations will be used to present a description of the sequence of the solidification events in these droplets.

9:40 AM
Three Dimensional Analysis of the Pore Structure in a Bioactive Glass Foam: *Robert C. Atwood*[1]; Julian R. Jones[1]; Peter D. Lee[1]; [1]Imperial College London, Matls., Prince Consort Rd., London SW7 2BP UK

Bioactive 3D scaffolds with potential for tissue engineering applications were fabricated by foaming a sol-gel derived bioactive glass which is known to bond to bone. This is due to the formation of a hydroxycarbonate apatite layer (similar to the apatite in bone) on the glass surface on contact with body fluid. The effectiveness of these open cell structures to act as a scaffold depends upon many different features, both chemical and structural. In this paper the effect of altering the sintering temperature upon the structural aspects is investigated using x-ray microfocal tomography. This technique allows the three dimensional visualization of several aspects of the structure: pore size and the size and number of connections between pores. These features are critical for the extracellular fluid to enter the structure and transport growth enhancing agents, as well as to the mobility of cells such as osteoblasts to enter the structure and deposit tissue. Deriving measurements from the data is more difficult and a novel computational method for both detecting and measuring them was developed.

10:00 AM Break

10:20 AM
Quantification of Rapid Solidification Events in Al-Cu Powders: *Arvind Prasad*[1]; Hani Henein[1]; Kelly Conlon[2]; [1]University of Alberta, Advd. Matls. & Procg. Lab., Dept. of Chem. & Matls. Engrg., Edmonton Canada; [2]AECL, NRC, Chalk River Canada

X-Ray Tomography and Neutron Diffraction experiments were carried out on rapidly solidified Al5% and Al17% Cu rapidly solidified droplets. The images from the Tomography clearly showed the recalescence region within the droplets and the recalescence region occurring in the droplet was quantified. The Neutron Diffraction experiments were used to quantify the amount of second phase, $CuAl_2$, in these binary alloys. Combining the two results with the quantification of the volume percent of eutectic obtained by SEM, it was possible to calculate the amount of primary alpha formed during the different regimes of rapid solidification, namely Nucleation and Recalescence, Post Recalescence and Eutectic solidification. The presentation describes the quantification processes and the calculated results are discussed in terms of differences in alloy compositions.

10:40 AM
Three Dimensional Deformation Microstructure Under Microindents Measured Using Submicron Resolution X-Ray Structural Microscopy: *Wenge Yang*[1]; B. C. Larson[1]; G. M. Pharr[2]; G. E. Ice[1]; J. Z. Tischler[1]; J. D. Budai[1]; [1]Oak Ridge National Laboratory, Oak Ridge, TN 37831 USA; [2]University of Tennessee, Knoxville, & Oak Ridge National Laboratory, Oak Ridge, TN USA

High-brilliance synchrotron x-ray sources, high-precision x-ray focusing optics, and newly developed differential-aperture x-ray structural microscopy now provide the possibility to study mesoscale materials science with submicron resolution in three dimensions. This new 3d x-ray microscopy provides local crystal structure, orientation, and both elastic and plastic strain tensors. In this talk, we will focus on the measurements of local lattice rotation and the local lattice curvature in terms of the geometrically necessary dislocation (GND) density and dislocation tensors under spherical micro-indents in single crystal Cu. Microstructures measured using the x-ray microdiffraction technique for maximum loads from 12.5 mN to 400 mN show well defined local lattice rotation and GND patterning structure, which for the first time explores the evolution of deformation non-destructively. The deformation microstructures will be compared and discussed in relation to deformation modelling possibilities.

11:00 AM
Computer Tomography 3-D Imaging of the Metal Deformation Flow Path in Friction Stir Welding: *Judy Schneider*[1]; Ronald Beshears[2]; Arthur C. Nunes[3]; [1]Mississippi State University, Mechl. Engrg. Dept., PO Box ME, Mississippi State, MS 39762 USA; [2]NASA-Marshall Space Flight Center, Non-Destructive Evaluation Team, ED32, Huntsville, AL 35812 USA; [3]NASA-Marshall Space Flight Center, Matls. Processes & Mfg. Dept., ED33, Huntsville, AL 35812 USA

In friction stir welding, a rotating threaded pin tool is inserted into a weld seam and literally stirs the edges of the seam together. This solid-state technique has been successfully used in the joining of materials that are difficult to fusion weld such as aluminum alloys. To determine optimal processing parameters for producing a defect free weld, a better understanding of the resulting metal deformation flow path is required. Marker studies are the principal method of studying the metal deformation flow path around the FSW pin tool. In our study, we have used computed tomography (CT) scans to reveal the flow pattern of a lead wire embedded in a FSW weld seam. At the welding temperature of aluminum, the lead becomes molten and thus tracks the aluminum deformation flow paths in a unique 3-dimensional manner. CT scanning is a convenient and comprehensive way of collecting and displaying tracer data. It marks an advance over previous more tedious and ambiguous radiographic/metallographic data collection methods.

11:20 AM

A 3D Measurement Procedure for Internal Local Crack Driving Forces via Synchrotron X-Ray Microtomography: *Hiroyuki Toda*[1]; *Toshiro Kobayashi*[1]; Ian Sinclair[2]; Kern Hauw Kohr[2]; Jean-Yves Buffière[3]; Eric Maire[3]; Peter Gregson[2]; [1]Toyohashi University of Technology, Dept. of Production Sys. Engrg., 1-1, Hibarigaoka, Tempaku, Toyohashi, Aichi 441-858 Japan; [2]University of Southampton, Sch. of Engrg. Scis., Highfield, Southampton, Hant SO17 1BJ UK; [3]INSA de Lyon, GEMPPM UMR CNRS 5510, 20, Av. A Einstein, Villeurbanne, Cedex 69621 France

Synchrotron X-ray microtomography has been utilized for the in-situ observation of fatigue crack opening/closure during load cycles. High-resolution phase contrast imaging technique has enabled the reconstruction of clear crack images together with the details of microstructural features. Physical displacements of micro-pores in a crack-tip stress field are used to obtain local mixed-mode crack driving forces along a crack front, and its feasibility is confirmed. Complicated crack closure behaviour are observed due to the combined effects of local modes II and III displacements. The technique used provides a highly effective way of assessing local crack driving forces together with supplementary ways of verifying and interpreting it by visualising and quantifying various forms of crack-tip shielding behaviour. The proposed technique is clearly advantageous compared to the limited procedures available in the current literature, where detailed internal information can only be achieved for limited types of material.

11:40 AM

FeatureView: A 3D Microstructure Extraction and Visualization Tool: *Mahnas Jean Mohammadi-Aragh*[1]; Sean Bernard Ziegeler[1]; Robert J. Moorhead[1]; Kelly Parmley Gaither[2]; [1]Mississippi State University, GeoResources Inst. - VAIL, PO Box 9627, Mississippi State, MS 39762 USA; [2]University of Texas, TX Advd. Computing Ctr., Austin, TX 78758 USA

Realistic, large-scale simulations generate massive amounts of data from which information is extracted to provide analysis. The ability to provide useful, pertinent information requires that data sets be analyzed using feature detection and extraction techniques. These features must then be quantified. To solve this problem, we developed FeatureView, a front-end visualization tool that can be used to analyze microstructures. It utilizes several algorithms, which can also be run independently in batch mode to preprocess large datasets. Currently, a prototype histogram-entropy threshold algorithm automatically segments objects for display in FeatureView. The objects are compactly represented using our 3D Line Segment Coding method. In addition, an isosurface is generated for each object and preliminary statistics, such as volume and surface area, are calculated.

Advancements in Mechanical Property Characterization at the Micro- and Nano-Scale: Development and Application of Mechanical Property Characterization Methods I

Sponsored by: TMS - Structural Materials Division

Program Organizers: Mike Uchic, Air Force Research Laboratory, Dayton, OH 45433-7817 USA; Kevin J. Hemker, Johns Hopkins University, Department of Mechanical Engineering, Baltimore, MD 21218 USA; Marc Zupan, University of Maryland, Baltimore, MD 21250 USA

Tuesday AM — Room: Mardi Gras Ballroom B
September 28, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Marc Zupan, University of Maryland, Dept. of Mechl. Engrg., Baltimore, MD 21250 USA; Ioannis Chasiotis, University of Virginia, Dept. of Mechl. & Aeros. Engrg., Charlottesville, VA 22904 USA

8:30 AM Opening Remarks

8:35 AM Invited

High Temperature Tensile Testing at the Microscale: *William N. Sharpe*[1]; [1]Johns Hopkins University, Dept. of Mechl. Engrg., 3400 N. Charles St., Baltimore, MD 21218 USA

There is always a need for materials with good mechanical properties at high temperature, even when the components are small. Examples of applications in microelectromechanical systems (MEMS) are resistively heated polysilicon actuators and sensors/actuators used in jet engines. This paper presents an overview of the testing challenges involved and some details on three methods. Polysilicon tensile specimens with a gage cross-section 3.5 µm by 50 µm are tested in a small furnace including a quartz window. Force is applied via a silicon carbide fiber glued to the end of the specimen and attached to a load cell on a piezoelectric actuator. Strain is measured by laser-based interferometry from gold lines spaced 250 µm apart on the specimen, and the maximum temperature was 250°C. Young's modulus decreases slightly with increasing temperature, but the fracture strength of this brittle material does not change. Larger polysilicon specimens - 3.5 µm by 600 µm in the gage section - are heated resistively. This makes it easier too reach high temperatures (700°C maximum), but requires platinum markers instead of gold ones. Temperature is measured via an optical pyrometer, and the specimen is again extended with a piezoelectric actuator. Brittle polysilicon begins to show inelastic behavior at ~ 475°C and is quite ductile at 670°C. Creep strain can be measured for durations of days, and the coefficient of thermal expansion is found to be somewhat larger than for single crystal silicon. Silicon carbide is a good candidate for MEMS at high temperatures, and strength measurements at 1000°C are being made to evaluate fabrication processes. These tensile specimens have gage cross-sections of ~ 100 µm by 200 µm and are heated in a closed furnace. Ceramic grips and supports hold the specimens, and the load is transferred out of the furnace with a coated wire. Initial results show no decrease in strength at the high temperature.

9:05 AM

Characterization of the Tensile Behavior of Single Crystal and Polycrystalline Ni-Base Superalloys at Elevated Temperatures Using Miniaturized Electro-ThermoMechanical Testing: *Sammy Tin*[1]; Yi Shen[1]; Bryan Roebuck[2]; [1]University of Cambridge, Dept. of Matls. Sci. & Metall., Pembroke St., Cambridge CB2 3QZ UK; [2]National Physical Laboratory, Matls. Ctr., Teddington, Middlesex TW11 0LW UK

Current methods of assessing and characterizing the mechanical response of high performance aerospace materials at elevated temperatures require substantial lead times and resources even when dealing with small-scale specimens. A miniature thermomechanical test unit developed by the National Physical Laboratory, UK (NPL) and INSTRON has been utilized to rapidly evaluate the mechanical response materials using sub-millimeter sized specimens. Coupled with the small specimens, the ETMT unit provides the capability to simulate tensile/compression deformation, thermo-mechanical fatigue, fatigue and creep deformation over a wide range of temperatures. Even with small quantities of material, this enables full and detailed characterization of the bulk mechanical properties. For the present investigation, the ETMT unit has been used to measure the tensile properties of polycrystalline superalloy IN718 and a number of experimental single crystal superalloys over a range of temperatures. These results are compared with those from conventional testing methods and the potential applications of the new testing unit are discussed.

9:25 AM

Micro-Mechanical Characterization of As-Deposited and Thermally Cycled Bond Coat Layers in Thermal Barrier Coating Systems: *Daniel T. Butler*[1]; Kevin J. Hemker[1]; Richard Wellman[2]; John Nicholls[2]; Michael D. Uchic[3]; [1]Johns Hopkins University, Dept. of Mechl. Engrg., 3400 N. Charles St., Baltimore, MD 21218 USA; [2]Cranfield University, Sch. of Indust. & Mfg. Sci., Bedford, Cranfield MK43 OAL UK; [3]Air Force Research Laboratory, Matls. & Mfg. Direct., AFRL/MLLMD, 2230 Tenth St., WPAFB, OH 45433-7817 USA

With typical length scales on the order of tens or hundreds of microns, characterization of as-deposited and thermally cycled thermal barrier coating (TBC) systems employed in aerospace applications poses a significant technological challenge. The aim of determining accurate mechanical properties over the full range of in-service temperatures, more specifically up to approximately 1100°C, adds an additional level of complexity. This talk describes two novel techniques developed to specifically address these challenges. First, the application of a computer-controlled microsample testing machine and load cell to perform micron-scale tensile tests of bow-tie shaped specimens prepared from bond coat layers is discussed. Using this test methodology, strength and creep data of RuAl bond coats are determined over a range of service temperatures. Alternately, a Focused Ion Beam (FIB) is employed to fabricate micron-scale compression samples from identical bond coat layers. A nanoindenter equipped for high temperature applications and fitted with a flat tip is employed to perform the subsequent compression tests over a narrower range of temperatures. Through the application of this technique we also determine elevated temperature mechanical properties of various TBC layers.

9:45 AM

Fatigue and Yield of Micron-Scale Titanium Under Torsion: *Marco F. Aimi*[1]; Masa P. Rao[2]; Noel C. MacDonald[2]; [1]University of California, Matls., Santa Barbara, CA 93106-5050 USA; [2]University of California, Mechl. & Environ. Engrg., Santa Barbara, CA 93106-5070 USA

The effect of reducing length scales on the mechanical properties of materials is of particular importance in Microelectromechanical Systems (MEMS). The recent development of MEMS created from bulk titanium substrates gives an opportunity to investigate the role of decreasing size on the fatigue and yield properties of titanium. To better understand these effects, the Metal Anisotropic Reactive Ion etching with Oxidation (MARIO) process is used to fabricate an array of micron-scale torsional beams with varying widths from 1 - 10 mm. These beams are tested for yield through the application and measurement of a torsional load and displacement using a Nanoindeneter. The testing of fatigue is preformed using the electrostatic attraction of the loading plate to underlying electrodes and is measured using laser doppler vibrometry. Results of both the fatigue and yield tests will be presented along with the details of the fabrication process.

10:05 AM Break

10:25 AM Invited
Mechanical Behavior of Nano-Grained Thin Metal Films: Aman Haque[1]; Jong Han[1]; *Taher Saif*[1]; [1]University of Illinois, Dept. of Mechl. & Indust. Engrg., 1206 W. Green St., Urbana, IL 61801 USA

Thin metal films are extensively used in electronics and micro/nano mechanical systems. These nano scale metal structures are typically polycrystalline in nature with abundant grain boundaries. The fundamental role of size scale in determining the thermomechanical properties of nano metallic structures is not yet fully understood, a study that is challenged by the limitations of the instrumentation that allows testing nano scale specimens. We have developed a new micro mechanical experimental method to study the stress-strain response of free standing thin metal films with thickness 20 nm or higher, in-situ in TEM and SEM. We employed the microinstrument to study Aluminum and gold films with thicknesses of 30-400nm, and with the corresponding grain sizes of 10-200nm. We find, as grain size decreases, (1) elastic modulus decreases, (2) metals show non-linear elastic response with small plastic deformation, and (3) yield stress increases, reaches a maximum value and then decreases with further decrease of grain size. In-situ observation of Al samples shows little dislocation activity in grains with size 100nm or less even at high stresses, which point to a grain boundary based mechanism for nano grained metal deformation. It appears that there is a shift of the deformation mechanism as grain size decreases: at small grain size dislocation slip ceases to operate and deformation is contributed by grain boundary mechanisms, whereas as grain size increases, dislocation dynamics overwhelms the grain boundary mechanisms. At the transition size, where the grains are small so that dislocation dynamics is energetically unfavorable, but not small enough for grain boundaries to assist in deformation, metal may show highest strength. For Al, this critical grain size seems to be around 50 nm from our experimental observations, close to 20-30 nm predicted by theory. Below this transition size scale, metals become softer and they lose strain gradient strengthening due to lack of dislocations.

10:55 AM
Tension/Compression Asymmetry, Anisotropy and Size Effects in the Plastic Deformation of Ti-6242 Single Colonies: *David Matthew Norfleet*[1]; Michael J. Mills[1]; Michael D. Uchic[2]; Mike F. Savage[3]; Joe Tatalovich[1]; [1]Ohio State University, Matls. Sci. & Engrg., 2041 College Rd., 477 Watts Hall, Columbus, OH 43210 USA; [2]Air Force Research Laboratory, Matls. & Mfg. Direct., Wright Patterson AFB, Dayton, OH 45433 USA; [3]Pratt & Whitney, E. Hartford, CT 06108 USA

The constant strain rate deformation behavior of individual alpha/beta colonies of the titanium aeroengine alloy Ti-6Al-2Sn-4Zr-2Mo-0.1Si (composition in wt.%) has been studied through an ultra small-scale compression technique. Using a FEI Dual Beam Focused Ion Beam, cylindrical compression samples were micromachined into the grip-ends of sub-millimeter-scale samples that previously had been tested in tension. Thus, one goal of the work is determine if a pronounced tension/compression asymmetry exists for these single colony crystals, while performing the test on the same samples and using the same deformation axis. Six single colony crystal orientations are being explored, associated with single slip in the HCP alpha phase along the three distinct a-type slip systems on both basal and prism planes. The compression samples, having diameters ranging from 10 to 35 microns, were mechanically tested using an MTS Nano Indenter XP fitted with a flat tip to apply uniaxial compression at a constant strain rate. The effect of sample size on the flow properties will be discussed. The resulting data will be correlated with tensile results, and TEM studies will be presented.

11:15 AM
Experimental Techniques for Scale-Specific Tension Testing of Aerospace Alloys: *Robert J. Thompson*[1]; Kevin J. Hemker[1]; William N. Sharpe[1]; [1]Johns Hopkins University, Dept. of Mechl. Engrg., 3400 N. Charles St., Baltimore, MD 21218 USA

The evaluation and knowledge of mechanical properties on the local level is a major factor governing the implementation of new aerospace alloys. Local property analysis of materials and structures, as opposed to average measures, enables designers to more efficiently select a material for a given application. For this investigation, a novel microsample fabrication and testing procedure is employed to gather small scale and scale-specific material properties. Microsample tensile specimens are created with laser and chemical milling procedures which generate the general sample geometry from a piece of bulk material. After polishing, a suitable grain or phase is located in the gauge section. This structure is then isolated using focused ion beam milling such that it represents the lowest value of cross-sectional area for the gauge section. From this, a uniaxial microsample tension test is performed to extract the local material properties. Tests run on titanium and nickel alloys are used to illustrate the methodology and utility of this approach.

Applications of Orientation Microscopy Techniques to Phase Transformations: Ferrous Alloys I

Sponsored by: TMS - Materials Processing & Manufacturing Division, TMS - MPMD-Phase Transformations Committee-(Jt. ASM-MSCTS)
Program Organizers: Robert E. Hackenberg, Los Alamos National Laboratory, Materials Science and Technology Division, Los Alamos, NM 87545 USA; Richard W. Fonda, Naval Research Laboratory, Washington, DC 20375 USA; Milo V. Kral, University of Canterbury, Department of Mechanical Engineering, Christchurch New Zealand

Tuesday AM — Room: Mardi Gras Ballroom C
September 28, 2004 — Location: Marriott New Orleans Hotel

Session Chair: Robert E. Hackenberg, Los Alamos National Laboratory, Matls. Sci. & Tech. Div., Los Alamos, NM 87545 USA

8:30 AM Invited
Crystallographic Relationships Between FCC and BCC Crystals During Transformation Under Equilibrium Conditions: A Meteorite Study Using EBSD: John J. Jonas[1]; *Youliang He*[1]; Stephane Godet[1]; [1]McGill University, Matls. Engrg., 3610 Univ. St., Montreal, QC H3A 2B2 Canada

Metallic meteorites cool at the rate of a few degrees per million years, thus providing ideal materials for the study of phase transformations under equilibrium conditions. Such cooling rates cannot of course be reached under laboratory conditions. During the extremely slow cooling stage, the initial FCC taenite (Fe-7.9%Ni) transforms into the BCC kamacite, where the latter has a lower concentration of Ni (<7.5%). This enriches the taenite in Ni (to >25%), so that some of the latter is retained on cooling, a phenomenon that makes it possible to measure the orientations of the parent phase before transformation. In this study, a piece of the Gibeon (Namibia) iron meteorite was investigated by means of optical microscopy and Electron Backscatter Diffraction (EBSD) techniques. The orientations of both parent and product phases were measured and the misorientation relationships are represented in Rodrigues-Frank (RF) space. From the orientation of a particular taenite crystal, the crystallographic orientations of the kamacite crystals can be predicted according to the Bain, Kurdjumov-Sachs (KS) and Nishiyama-Wassermann (NW) transformation relationships. A comparison of the predicted and measured relationships reveals that the Bain relationship is never found; the KS and NW relationships are both observed and there is a continuous distribution of misorientations between the exact KS and NW positions. This conclusion holds for both the large Widmanstätten kamacite (BCC) lamellae as well as the tiny kamacite grains in the plessite (eutectoid) regions of the meteorite investigated. The significance of the continuous spread of misorientations (between KS and NW) is discussed briefly.

9:00 AM Invited
A Study of Plessite Structures in the Gibeon Meteorite: *Bevis Hutchinson*[1]; Joacim Hagström[1]; [1]Swedish Institute for Metals Research, Drottning Kristinas väg 48, Stockholm SE-11428 Sweden

Gibeon is an example of a fine octahedrite meteorite having a structure of Widmanstätten kamacite (ferrite) separating islands of plessite, a two phase mixture of kamacite and taenite (austenite). Very little attention has been accorded to plessite structures in the literature but these are extremely variable in orientation, form and scale and lend themselves ideally to examination using EBSD and orientation imaging. The original structure prior to transformation was a single crystal of fcc taenite which has transformed to a complete spread of variants of kamacite having orientation relationships ranging between Kurdjumov-Sachs and Nishiyama-Wassermann. Most plessite consists of kamacite with subboundaries and islands of retained tainite at these boundaries. Kamacite subgrains vary in scale from >100 to <1 micrometre apparently depending on the temperature at which the original taenite decomposed. Some plessite islands have undergone recrystallisation and within these may exist different families of needle-shaped taenite particles having small systematic misorientations.

9:30 AM
EBSD of Proeutectoid Cementite: *Milo V. Kral*[1]; [1]University of Canterbury, Mechl. Engrg., PO Box 4800, Ilam, Christchurch New Zealand

The crystallography and morphology of proeutectoid cementite precipitates were studied in an isothermally transformed Fe-1.3%C-12%Mn steel via Electron Backscattered Diffraction (EBSD) and scanning electron microscopy. Widmanstatten precipitates developed different morphologies depending on the orientation relationship obtained with the matrix austenite. Grain boundary cementite precipitates develop with complex variations of a morphology that can be described as fern-like dendrites growing preferentially within and along austenite grain boundaries. EBSD pattern analysis showed that most of the grain boundary cementite precipitates approximated one of the known cementite-austenite crystallographic orientation relationships (OR) with at least one of its adjacent austenite grains. Occasionally, the grain boundary cementite exhibited an OR that achieved 'best fit' directions between the cementite and austenite in both adjacent austenite grains.

9:55 AM Break

10:25 AM Invited
Morphology and Crystallography of Martensite and Bainite in Ferrous Alloys: *Tadashi Maki*[1]; [1]Kyoto University, Dept. of Matls. Sci. & Engrg., Sakyo-ku, Kyoto 606-8501 Japan

Various effects such as alloying elements, transformation temperature, austenite grain size and ausforming on the morphology and crystallography of lath martensite and bainite in Fe-C and Fe-Ni alloys were studied in detail mainly by TEM observation and EBSP technique. In Fe-C alloys, the sizes of both packet and block in lath martensite decrease with an increase in the carbon content. In low carbon steels (0-0.38%), a block contains two groups (sub-block) of laths which are of the two K-S variants with a misorientation of about 10 degree. On the other hand, in the high carbon alloy (0.61%C), a block consists of laths with a single K-S variant. The size of block markedly decreases by the ausforming and the refinement of austenite grain size. Similar results of upper bainite are also shown.

10:55 AM
Combined Orientation and Phase Contrast Imaging of Precipitates in 9-12% Cr Steels: *Bernhard Sonderegger*[1]; Stefan Mitsche[2]; Horst Cerjak[1]; [1]Graz University of Technology, Inst. for Matls. Sci., Welding & Forming, Kopernikusgasse 24, Graz, Austria A- 8010 Austria; [2]Graz University of Technology, Rsch. Inst. for Electron Microscopy & Fine Struct. Rsch., Steyrergasse 17, Graz, Austria A-8010 Austria

9-12% chromium steels are well established materials for high temperature components in ultra efficient power plants. An important parameter for the creep resistance of these steels is the formation and interaction of different precipitate populations within the martensitic/ ferritic matrix. In this work, EBSD studies were carried out on samples of the European COST steel CB8, which had been creep loaded at 923K for up to 16000h. These studies were supplemented by phase contrast images at the same sample positions in order to detect Mo- rich Laves phase. This combination of measurement techniques gives the full information of frequency and size of the precipitates depending on the orientation and misorientation of neighbouring subgrains. With this information, formation and growth of precipitates can be characterised under local conditions in the course of in-service exposure.

11:20 AM
Susceptibility of Stainless Steels to Transformation Induced Plasticity: *C. T. Necker*[1]; M. C. Mataya[1]; D. K. Matlock[2]; [1]Los Alamos National Laboratory, MST-6, Los Alamos, NM 87545 USA; [2]Colorado School of Mines, Dept. of Metallurgl. & Matls. Engrg., Golden, CO 80401 USA

Certain stainless steels as well as some low/medium carbon steels exhibit a TRansformation Induced Plasticity (TRIP) wherein austenite or retained austenite, depending on both composition and prior thermomechanical processing, undergoes a strain-induced martensitic transformation. The transformation locally increases the material toughness, decreases the propensity for localized necking and forces surrounding material to accommodate additional plastic deformation. 301, 304 and 305 stainless steels differ in their susceptibility to this strain induced phase transformation based on the differing degrees of austenitic stabilizing elements. The degree of transformation in thin sheet, deformed under unaxial tensile conditions, is macroscopically tracked via a ferrite scope and X-ray diffraction. The development of the microstructure and transformation textures is monitored using an Electron BackScatter Pattern (EBSP) recognition system. As expected, the 301 alloy exhibits greater degree of transformation as a function of strain as compared to the 304 alloy. The additionall alloy content of 305 stainless all but eliminates the ability of this alloy to undergo the transformation.

Computational Microstructure Evolution in Steel: Recrystallization and Grain Growth

Sponsored by: TMS - Structural Materials Division, TMS - EMPMD/ SMD-Chemistry & Physics of Materials Committee, TMS - MPMD-Computational Materials Science & Engineering-(Jt. ASM-MSCTS)
Program Organizers: Koenraad G.F. Janssens, Sandia National Laboratories, Materials and Process Modeling, Albuquerque, NM 87185-1411 USA; Mark T. Lusk, Colorado School of Mines, Mechanical Engineering Program, Division of Engineering, Golden, CO 80401 USA

Tuesday AM — Room: La Galerie 4
September 28, 2004 — Location: Marriott New Orleans Hotel

Session Chair: Koenraad G.F. Janssens, Sandia National Laboratories, Albuquerque, NM 87185 USA

8:30 AM Invited
Simulation of Grain Growth in Fe-3Si: *Anthony D. Rollett*[1]; Tricia Bennett[1]; Dierk Raabe[2]; [1]Carnegie Mellon University, Matls. Sci. & Engrg., 5000 Forbes, Pittsburgh, PA 15213 USA; [2]Max-Planck-Institut fuer Eisenforschung, Abteilung Mikrostrukturphysik und Umformtechnik, Max-Planck-Str. 1, Duesseldorf 40237 Germany

Maps obtained from automated electron back-scatter diffraction (EBSD) have been mapped pixel-for-pixel into Monte Carlo simulations of grain growth. Simulations of grain growth have been performed to explore the potential for abnormal growth, especially of the Goss component. Significant variation in texture development has been found based on different assumptions about the key grain boundary properties in iron, i.e. energy and mobility. The literature is inconsistent and incomplete in this area, which appears to leave room for reinterpretation of the data.

9:10 AM
An Analysis of the Strain Dependent and Strain Independent Recrystallisation Regions of Various Grades of Hot Worked Steel: *Mark Robert Cartmill*[1]; Matthew Barnett[1]; Peter Hodgson[1]; Ronald Gloss[2]; [1]Deakin University, Engrg. & Tech., Pigdons Rd., Geelong, VIC 3217 Australia; [2]Bluescope Steel, Western Port Hot Strip Mill, PO Box 1, Hastings, VIC 3915 Australia

The transition from strain dependent to strain independent recrystallisation exerts a major influence upon the softening behaviour of steel following hot deformation. This transition occurs at a characteristic strain ε^*, which depends strongly upon both strain rate and temperature. In the present work, the strain dependent and strain invariant recrystallisation regions are examined both mechanically and metallographically for a range of steel alloys. It has been found that at low values of Z, ε^* tends to consistently coincide with peak strain, whereas at higher Z values ε^* occurs at much higher strains then the peak. The influence of precipitation on ε^* for two grades of HSLA steel has also been examined and a model developed for the prediction of ε^* as a function of grain size and Zener-Hollomon parameter.

9:30 AM Cancelled
Recrystallization of Austenite During and Following Hot Deformation: Ali Dehghan-Manshadi[1]; *Matthew Robert Barnett*[1]; Peter Damian Hodgson[1]; [1]Deakin University, Sch. of Engrg., Pigdons Rd., Geelong, VIC 3217 Australia

9:50 AM
Monte Carlo Simulation of Elongated Recrystallized Grains in Steels: *Kaneharu Okuda*[1]; Anthony D. Rollett[2]; [1]JFE Steel Corporation, Steel Rsch. Lab. Sheet Products Rsch. Dept., 1 Kawasaki-cho, Chuo-ku, Chiba 260-0835 Japan; [2]Carnegie Mellon University, Matls. Sci. & Engrg. Dept., 5000 Forbes Ave., Wean Hall 4315, Pittsburgh, PA 15213-2890 USA

A Monte Carlo simulation technique was employed to model special recrystallized grains in steels; batch-annealed pancake grains, or Nb bearing elongated ones. The first simulation focused on grain boundary characters. Lower misorientations between matrix and recrystallized grains made the recrystallized grains abnormally grow into the other matrix grains. However, if matrix grains had a large difference in stored energy at a boundary, the movement of the grain boundary could be hindered; the recrystallized grain cannot grow into the matrix. Hence elongated grains could be obtained on the special orientational relationship at the boundary without dispersed fine particles. Then particle pinning was examined. The particles retards recrystallization only on a condition with low stored energies; the largest grain was obtained on the critical condition for recrystallization. In this way, if nucleation sites are quite restricted, larger elongated grains could be obtained.

10:10 AM Break

10:30 AM Invited
Multi-Scale Life Cycle Modeling of Steel Components at Caterpillar: *Leo Chuzoy*[1]; [1]Caterpillar

Abstract not available.

11:10 AM
Microstructure Modeling of Vanadium Microalloyed Steels: *Oscar Vasquez*[1]; Robert Pow[1]; Leo Frawley[2]; Matthew Barnett[1]; Peter Hodgson[1]; [1]Deakin University, Sch. of Engrg. & Tech., Pigdons Rd., Waurn Ponds, Geelong, Victoria 3217 Australia; [2]Smorgon Steel Ltd., Quality Assurance, Dohertys Rd., Laverton, Melbourne 3026 Australia

The use of microalloyed steels in particular alloying with vanadium, has increased dramatically over recent years as higher strengths and lower processing costs are achieved. Understanding the development of the austenitic microstructure during hot rolling is essential to optimize the rolling schedule so that the resulting mechanical properties satisfy quality and performance standards. Development of a refined austenite microstructure leads to a refined ferrite/pearlite microstructure, while the level of precipitation hardening is also linked to the transformation process. The effect of various temperatures and rolling schedules in relation to recrystallisation kinetic was examined for two types of steels: a vanadium microalloyed steel and a low carbon steel. Torsion tests were carried out for temperatures from 900°C-1100°C and strain rates from 0.1-10. Determination of the rate of recrystallisation and recrystallised grain size was undertaken for both steel compositions. The role of the microalloying element on the recrystallisation, transformation and level of precipitation was determined. All of this information was used to construct a metallurgical model of the rolling process.

11:30 AM
Phase Field Simulation of Transformation Kinetics in a Low Carbon Steel: *Cheng-Jiang Huang*[1]; Dian-Zhong Li[2]; David John Brown[1]; [1]University College, Dept. of Mechl. Engrg., Belfield, Dublin 4 Ireland; [2]Chinese Academy of Sciences, Inst. of Metal Rsch., 72 Wenhua Rd., Shenyang, LiaoNing 110016 China

Decomposition of austenite in steels has been modelled by many scientists, using various methods, at different length scales. Recent real-time X-ray observation has revealed several complex grain growth modes, quite different from the prediction of Avrami-type equations. Some grains even shrank during the "grain growth" stage (S.E.Offerman et al, Science, 298, 2002, 1003-1005). The experimental observations have not been revealed by models published to date. The phase field method is becoming increasingly popular as a means of simulating phase transformation. It has some important features that are lacking in other methods, including the general ability to predict the movement of many complex interfaces. The authors have re-examined the austenite-ferrite transformation in steels, using phase field simulation, comparing the results with the most recent real-time X-ray observation. Special emphasis was placed on the complex growth modes of individual grains. This study will lead to the revelation of some new details of this important transformation.

Continuous Casting Fundamentals: Mold Fluid Flow and Water Spray Cooling

Sponsored by: AIST, TMS, AIST - Division VI, AIST - Division VII, TMS - MPMD-Solidification Committee, TMS - MPMD/EPD-Process Modeling Analysis & Control Committee
Program Organizers: Brian G. Thomas, University of Illinois, Department of Mechanical and Industrial Engineering, Urbana, IL 61801 USA; Michael Byrne, International Steel Group, Homer Research Labs, Bethlehem, PA 18016 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Tuesday AM — Room: Grand Ballroom M
September 28, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Mike Byrne, International Steel Group, Homer Rsch. Labs, Bethlehem, PA 18016 USA; Brian Thomas, University of Illinois, Dept. of Mechl. & Indust. Engrg., Urbana, IL 61801 USA

8:30 AM
A Physical Model Study for the Two-Phase Flow in a Continuous Casting Mold: *Rodolfo Davila Morales*[1]; [1]IPN-K&E Technologies, Metall., Ed, 7, UP Zacatenco-Lindavista, And. 8 de Fdo. Amilpa No. 7 UCTM-El Risco, Mexico D.F. 07090 Mexico

Two-phase flow in a water model of a continuous casting mold is studied using Particle Image Velocimetry. At low gas-loads (mass flow rate of gas/mass flow rate of liquid) fluid flow patterns of phases, gas and liquid, are different and with increases of this parameter both flow fields become similar. In the liquid phase, angles of the jet root (in front of the SEN's ports) and jet core (main jet-body)are complex functions of the gas flow and casting rates. The first is decreased well below the angle of the SEN's port and the second is increased well above the same angle for all gas-loads. The jet-root angle increases, from small values, while the jet core-angle observes a maximum with the gas flow rate at any casting rate. The jet angle approaches to the angle of the SEN's port at high flow rates. Accumulation of bubbles is observed in the mold cavity when the casting rate is high at low or high flow rates of gas. Averaged bubble sizes depend on the coalescence-breakup kinetics, which vary with the gas load. Liquid entrainment by gas to the flux is greatly increased with the casting rate even at low gas-loads. Further understanding of the two-phase flow dynamics should be attained in order to improve boundary conditions of mathematical models.

8:55 AM
Inclusion Removal by Bubble Flotation in Continuous Casting Mold: *Lifeng Zhang*[1]; Jun Aoki[1]; Brian G. Thomas[1]; [1]University of Illinois, Mechl. & Indust. Engrg., 345 Mech. Engrg. Bldg., 1206 W. Green St., Urbana, IL 61801 USA

The attachment probability of inclusions on a bubble surface is investigated based on fundamental fluid flow simulations, incorporating the inclusion trajectory and sliding time of each individual inclusion along the bubble surface as a function of particle and bubble size. Then, the turbulent fluid flow in a typical continuous casting mold, trajectories of bubbles and their path length in the mold are calculated. The inclusion removal by bubble transport in the mold is calculated based on the obtained attachment probability of inclusion on bubble and the computed path length of the bubbles. The results are important to estimate the significance of different inclusion removal mechanisms. This work is part of a comprehensive effort to optimize steelmaking and casting operations to lower defects.

9:20 AM Break

9:40 AM
Understanding the Role Water-Cooling Plays During Continuous Casting of Steel and Aluminum Alloys: *J. Sengupta*[1]; B. G. Thomas[1]; M. A. Wells[2]; [1]University of Illinois, Dept. of Mechl. & Indust. Engrg., 1206 W. Green St., Urbana, IL 61801 USA; [2]University of British Columbia, Dept. of Metals & Matls. Engrg., 6350 Stores Rd., Vancouver, BC V6T 1Z4 Canada

Water-cooling plays a major role in extracting heat from both the mold and solidifying metal during the continuous casting of steel and aluminum alloys and is characterized by complex boiling phenomena. Heat extraction rates during water-cooling, which has strong dependence on the metal surface temperature, can rapidly change with time as the strand cools down. Consequently, uncontrolled cooling may cause fluctuations in the temperature gradients inside the solidifying shell and generate tensile thermal stresses at the solidification front that can ultimately lead to the appearance of hot tears/cracks in the final product. This paper compares and contrasts the water-cooling techniques used for casting steel and aluminum and discusses their implications in terms of final product quality based on fundamental studies and predictive mathematical models. Finally, optimal practices for the control of cooling in casting processes for both steel and aluminum alloys are evaluated.

10:05 AM
Comparison of Impact, Velocity, Dropsize, and Heat Flux to Redefine Nozzle Performance in the Caster: *Kristy A. Tanner*[1]; [1]Spraying Systems Company, Heavy Industry, North Ave. at Schmale Rd., Wheaton, IL 60189 USA

Impact testing performed to empirically determine the impact and velocity of airmist nozzles used in continuous casting. Previous data from heat flux testing above Leidenfrost temperature is used to compare the affects of impact, velocity, dropsize on heat flux. A close look at the film boiling regime shows how impact and velocity can influence localized cooling. Flux distribution is compared to impact distribution to show different parameters defining traditional air mist nozzle performance.

10:30 AM
Spray Cooling Results of Air/Mist Spray Nozzles with Reduced Air Volumes: *Ken Kasperski*[1]; [1]Spraying Systems Co., North Ave. at Schmale Rd., Wheaton, IL 60189 USA

Continuous casters may benefit with reduced operating costs by decreasing air volumes required for air/mist spray nozzles in secondary cooling zones. Experimental results were examined to determine how heat transfer characteristics were affected by reductions of up to 25% of the air while water volumes were held constant. Mixing efficiencies of air and water were design variables considered. Minimum heat flux and Leidenfrost temperature values were compared at similar water flux density conditions.

10:55 AM
Using Particle Swarm Optimization Algorithm and Knowledge Database to Optimize Continuous Casting of the Steel Secondary Cooling Zone Water Flux and Casting Velocity: *Rongyang Wu*[1]; Hongji Meng[1]; Gouhui Mei[1]; Zhi Xie[1]; [1]Northeastern University of China, Shengyang, Liaoning 110004 China

The steel continuous casting process is a complex solidification process, and the process parameters, such as: casting velocity, each zone cooling water flux and so on, are very important to control the quality in continuous casting products. In this paper, solidification process is simulated using control volume method, to the continuous casting process nondifferentiable multiobjective optimal control, particle swarm optimization algorithm and steel metallurgy solidification knowledge database are used to optimize continuous casting secondary cooling zone water flux and casting velocity. The results of simulations performed using the mathematical model are validated against both experimental and literature results, and a good agreement are observed. Results can be produced for determining optimum settings of casting conditions, which are conducive to the best strand surface temperature and metallurgical length.

General Abstracts: Processing and Process Modeling

Sponsored by: AIST, TMS
Program Organizers: Dennis M. Dimiduk, Air Force Research Laboratory, Materials & Manufacturing Directorate, WPAFB, OH 45433 USA; E. Buddy Damm, The Timken Company, Canton, OH 44706-0930 USA; James C. Foley, Los Alamos National Laboratory, Los Alamos, NM 87545 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Tuesday AM — Room: Mardi Gras Ballroom A
September 28, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Patrick L. Martin, Air Force Research Laboratory, Matls. & Mfg. Direct., Wright-Patterson AFB, OH 45433-7817 USA; Jamie Tiley, Air Force Research Laboratory, Matls. & Mfg. Direct., Wright-Patterson AFB, OH 45433-7817 USA

8:30 AM
Growth of GaInSb Thin Films Using Hot-Wall Epitaxy: *Partha Bir Barman*[1]; [1]SLIET, Physics, Longowal, Sangrur, Punjab 148 106 India

Growth of GaInSb thin films was carried out using Hot wall Epitaxy system on high purity quartz glasses and high resistive silicon as a substrate. The source material for the film was grown using Vertical Bridgmen method. The epitaxial film were characterized using grazing angle x-ray diffraction method for crystallinity. XPS studies on the film showed non-stoichimetry compared to the bulk crystals used as source. Band gap measurement using FTIR confirms the energy-gap in the IR region, but doesn't exactly tally with the calculated theoritical values. SEM studies on the films were also carried out to estimate defect density on the grown films. Electrical characterisation of the film viz. Vander Pauw resistivity, Hall mobility and carrier concentration etc. mesurements are under progress and will be reported. Finally Au/GaInSb Schottky diodes were fabricated and electrically characterised for IR detectors. The study of interplay between the microstructure and the electrical properties of the thin film is in progress and will also be presented.

8:50 AM
The Etching Properties of an Fe-36%Ni Alloy as a Shadow Mask Material: *Toshiyuki Ono*[1]; [1]Nippon Mining & Metals Co., Ltd., Tech. Dvlp. Ctr., 3 Kurami, Samukawa, Koza, Kanagawa 253-0101 Japan

An Fe-36%Ni alloy which exhibits low thermal expansivity was chosen as a shadow mask material for high resolution CRTs. However, a defect, which looks like fine stripes along the rolling direction, has been a great concern to achieve high quality picture images. Investigations of etched surfaces by using SEM and EPMA revealed that irregular reflection of light at striae on etched hole walls is a cause of the defect. The striae were formed during etching by ferric chloride solution because of Ni segregation. Galvanically induced localized corrosion is considered to form the striae. Also a strong cubic texture was found to worsen the defect. Studies with EBSP showed that smooth surfaces of etched hole walls due to little difference in crystallographic orientation between neighboring grains enhanced the irregular reflection at the striae. Random crystallographic orientation of grains is preferable as well as reduction of Ni segregation to eliminate the defect.

9:10 AM
Prediction and Quality Control of Annealing in Bell Type Furnaces HICON/H_2: *L. I. Frantsenyuk*[1]; A. N. Fediainov[1]; [1]Research & Production Institute of Novolipetsk Iron & Steel Corporation Russia

The cost and productivity of annealing in bell type furnaces are determined by optimum combination of the configuration of coils stack and required annealing time to achieve the desired quality of annealed strip. The annealing time, as part of temperature program applied in a bell type furnace HICON/H_2, in turn, depends on the way account of weight and geometrical characteristics of a cold-rolled strip (thickness and width) at assignment of the temperature program. On the International conference «HICON/H_2-2000» was presented new model for calculation of heating and cooling times for coils of a steel strip in bell type furnaces HICON/H_2.[1] The program essentially differs from used before the statistical approach, and from completely theoretical model of the furnace, for which one complicating calculations and applying in calculations free (not exact) arguments is feature. In Research & Production Institute of Novolipetsk Iron & Steel Corporation was developed software for the prediction and quality control of annealing of a cold-rolled steel strip in bell type furnaces HICON/H_2. This software has two essential differences from other programs designed for the quantitative description of thermal fields of coils in stack. 1. It can be used not only for the prediction of thermal fields of coils (for example, in case of experimental program of annealing), but also for a quality control of completed annealing. One of examples of such control – when in case of failure heating system the temperature program was not properly executed, and it is necessary to estimate the drawing quality, obtained in result of the annealing, with purpose of applicable management of the product. 2. For prediction of annealing quality, temperatures of heating and inner cover spaces are accounted by dynamic model,[2] and for quality control these temperatures will equivalent with actual, registered by supervision system of bell type furnaces HICON/H_2 during annealing. The software was transmitted in technological service of a cold rolling shop for optimum management and quality control of annealing in bell type furnaces HICON/H_2. [1]G. Eckertsberger, Model to predict and supervise annealing and cooling times for EBNER HICON/H_2 bell annealers, Proc. int. conf. «HICON/H_2- 2000». [2]L. Ljung, T. Glad. Modeling of Dynamic Systems, Prentice Hall, Englewood Cliffs, N.J. 1994.

9:30 AM
Preparation of the Semi-Solid Blank of AZ91D Magnesium Alloy by SIMA Process: *Ze-Sheng Ji*[1]; Xiao-ping Zheng[1]; [1]Harbin University of Science and Technology, Dept. of Matls. Sci. & Engrg., Harbin, Heilongjiang Province 150040 China

This paper has studied the SIMA process used to prepare the semi-solid materials of AZ91D magnesium alloys, and given the technology, and investigated the influence of cold working rate, heating temperature and holding time on solid fraction, the size, distribution and shape of structures. The results show that: under the cold working condition, the SIMA process can produce the semi-solid materials of magnesium alloys of 55% minimum solid fraction after holding definite time on 570¡æ. The paper also analyzed forming mechanism of semi-solid materials of AZ91D magnesium alloys, and achieved conclusion: during heat treatment, structures would be re-crystallized. And the influence of re-crystallized structures is pronounced by cold working rate.

9:50 AM Break

10:00 AM
Supercomputer Application in Making Animation Software for Semiautogenous Grinding Mill: *Amol D. Joshi*[1]; [1]University of Utah, Metallurgl. Engrg., 1460 East 135 S., Rm. #412 Wbb, Salt Lake City, UT 84102 USA

Semiautogenous and ball mills are mainly used to grind mineral particle to increase the extraction yield. The mill operation cost is high because of its power consumptions, grinding balls & liners wearing and down time for changing liners. The main aim here is to come up with C animation code. This simulation software demands huge memory and processing time. Hence, this C version is parallelized using Message Passing Interface. This simulation code uses a numeric method known as the discrete element method. Overall motion of the charge is modeled by considering the forces generated at all points of collision made by individual balls and by following the motion of each and every ball. A force displacement law is applied at each contact and the Newton's second law of motion is used to calculate ball trajectories. Results of computations are verified with large amount of published industrial mill data for SAG mills and ball mills. They were very promising and accepted at industrial level.

10:20 AM
Effect of Immersion Orientation and Non-Uniform Fluid Flow on a Quenched Part During Liquid Quenching: *Mohammed Maniruzzaman*[1]; Darrell Rondaue[1]; Richard D. Sisson[1]; [1]Worcester Polytechnic Institute,

Matls. Sci. & Engrg., Mechl. Engrg. Dept., 100 Inst. Rd., Worcester, MA 01609 USA

Distortion and cracking of a metallic part quenched in a quenchant can be reduced greatly by improving quench uniformity. In this study, numerical experiments are performed to investigate the sensitivity of heat treatment response to non-uniformity of heat extraction rate of a steel plate quenched in liquid quenchant. The surface heat transfer coefficient (h) as a function of temperature is the input as a process variable to heat treatment simulation software DANTE/ABAQUS to predict the residual stress state and distortion of the plate. The results are analyzed as a ratio of h for front face to h for back face of the plate to determine the optimum h ratio for minimum distortion.

10:40 AM

A Mixed Reaction Kinetic Model for Gold Leaching With the Copper(II)-Ammonia-Thiosulphate System: *Gamini Senanayake*[1]; [1]Murdoch University, Extractive Metall. & Mineral Sci., A.J. Parker Ctr. for Hydrometall., Murdoch, Perth, WA 6150 Australia

The copper(II)-ammonia-thiosulphate system for leaching and recovery of gold has renewed research interest, mainly due to the environmental and economic benefits as well as the versatile nature of this non-cyanide route to process different types of material. The widely reported surface reaction mechanism for the leaching of gold with this lixiviant system involves the oxidation of gold by copper(II) to produce diammino complexes of gold(I) and copper(I). Due to the lower stability, these complexes are converted to thiosulphato complexes of gold(I) and copper(I). However, the analysis of literature data clearly shows the involvement of three redox reactions in the leaching process. The thermodynamic information on complexes of copper(II), copper(I) and gold(I), including the mixed ammonia-thiosulphate ligand complexes, are used to elucidate the surface reaction mechanism. Results based on the leaching data using different material and rotating gold discs are shown to be in reasonable agreement.

11:00 AM

Reduction of Zinc-Containing Metallurgical Residues in a Fluidized Bed Reactor: *S. M. Taghavi*[1]; M. Halali[1]; [1]Sharif University of Technology, Matl. Sci. & Engrg. Dept., Tehran Iran

In this report, the possibility of recovering zinc oxide from zinc oxide containing wastes has been studied. The ore was reduced in a fluidized bed furnace using a CO/CO_2 mixture as reducing agent. It has been shown that with increasing in temperature and time of reaction, recovery percent will increase, also when depth of bed increases, recovery percent will decrease. The best result was shown that zinc oxide content in product was more than %93.5.

11:20 AM

Statistical Study of Mo Recovery from Molybdenum Waste Catalyst: Seham Nagib Tawfic[1]; A. A. Ismail[2]; I. A. Ibrahim[2]; [1]Academy of Specific Study, Dept. Dvlp. of Tech., El-Nasr St. Abbaas El-Akkaad Corner, El-Nasr City Egypt; [2]Central Metallurgical R&D Institute, Box 87-Helwan, Helwan- Cairo City Egypt

Dissolution of molybdenum from molybdenum waste catalyst (MWC) that contain wt %: 42.79 Mo, 9.54 Fe, 4.9 Al, 8.68 SiO_2, 6 Na, and 1.5 Cr using different leaching agents such as H_2SO_4, HCl, and NaOH was carried out. It was found that, NaOH is the best leaching agent because it has the highest Mo recovery in combined with the lower Fe and Al dissolution than the HCl. Factorial design of experiments and application of statistical analysis on the results of leaching studies using NaOH were carried out. A regression equation for the dissolution of Mo was developed as a function of NaOH stoichiometric (S), L/S ratio (C, ml/g), and temperature (T, oC). All parameters were varied at two levels for designing experiments to estimate error.

High Strain Rate Deformation and Deformation Mechanisms of Structural Steels: Development and Application of High Strain Rate Properties

Sponsored by: AIST, AIST - Division VI

Program Organizers: James R. Fekete, General Motors Corporation, Metal Fabricating Division, Pontiac, MI 48341 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA; Benda Yan, Ispat Inland Steel, Product Applications, East Chicago, IN 46312 USA

Tuesday AM	Room: Grand Ballroom L
September 28, 2004	Location: Marriott New Orleans Hotel

Session Chairs: James R. Fekete, General Motors Corporation, Metal Fabricating Div., Pontiac, MI 48341 USA; Benda Yan, Ispat Inland Inc., Product Applications, E. Chicago, IN 46312 USA

8:30 AM

Strain Rate and Temperature Sensitivity of Trip Steel Sheets: *J. R. Klepaczko*[1]; A. Rusinek[1]; [1]University of Metz, Lab. of Physics & Mech. of Matls., UMR CNRS 75-54, Ile du Saulcy, 57045 Metz, Cedex France

Nowadays the TRIP steels are more extensively used in automotive applications. The high strength of those steels is due to the phase transformation, during plastic deformation. The strain hardening coefficient (), is not affected by the phase transformation for temperatures equal or higher then, but it reaches very high value at the low temperature close to (complete martensitic transformation without assistance of plastic deformation). Therefore, the stress evolution during plastic deformation is not only a function of strain rate and temperature but also of the rate of phase transformation which defines the transformation kinetics. The phase transformation is also affected by strain rate and temperature. This contribution reports not only the rate and temperature sensitivities but also the temperature measurements performed during plastic deformation at low and high strain rates. Such approach enables one to obtain complementary information on detection of phase transformation. In order to determine at the same time the temperature increments and plastic properties, an original experimental technique has been applied. A fast tensile hydraulic machine and an infrared camera which records the infrared radiation emitted during the process of plastic deformation were used. As a result, it is observed, for example, a very high gradient of temperature at low strain rates () increasing with the plastic of deformation. In dynamic loading, the latent heat due to phase transformation seems to be inexistent. In fact, when the strain rate and temperature are significant, > 1.0 s-1, the effects of phase transformation are suppressed. In conclusion, the tests have indicated a very complicated interplay of strain hardening, strain rate and temperature at different strain rates and initial temperatures. A set of constitutive relations are derived in a general form.

8:55 AM

Effect of Processing Parameters on the Deformation Behaviour of Low Carbon Dual Phase Strip Steels at High Strain Rates: *Nathan Daniel Beynon*[1]; Bryan Jones[2]; George Fourlaris[1]; [1]University of Wales, Engrg. Doctorate Ctr., Matls. Rsch. Ctr., Sch. of Engrg., Singleton Park, Swansea SA2 8PP UK; [2]Corus Strip Products UK, ECM2, Heol Cefn Gwrgan, Port Talbot Works, Port Talbot SA13 2EZ UK

This study primarily involved the production of dual phase microstructures in low carbon strip steels, via a modified steel-processing route, with the subsequent determination of the dynamic properties of the strip steels. Two commercial trial grades with compositions 0.094%C-0.155%Si-1.48%Mn-0.096%V and 0.096%C-0.13%Si-1.51%Mn-0.096%V, respectively were studied. The steels in the as received condition had a ferrite-pearlite microstructure and were subsequently subjected to intercritical annealing followed by rapid cooling/quenching. A series of ferrite-martensite-bainite structures were developed and the nominal yield strengths of these modified steel microstructures ranged from 280 to 450 MPa, with tensile strengths in the range of 600 to 800 MPa. Tensile and high-speed tensile testing at strain rates within the range of 0.001, 1 and 100s-1 were performed. The results showed that the yield/proof strength and tensile strength increased with increasing volume fraction of martensite and increasing strain rate. In particular, as far as the strain rate sensitivity and work hardenability properties are concerned, steels with a predominantly ferrite-martensite microstructure showed better performance than microstructures with additional non-equilibrium constituents, characterised in the main as bainite.

9:20 AM

Bake Aging of Structural Steel Grades: *Ben Clark*[1]; Peter Damian Hodgson[1]; [1]Deakin University, Pigdons Rd., Geelong, VIC 3217 Australia

The response of structural components to the bake cycle during automotive assembly is not well accounted for in crash models. The aim of this work is to quantify the bake hardening response of several trial structural steels. Steels examined included: commercial quality drawing steel, high strength low alloy (HSLA) 540 and 590 MPa, nano hardened 780 MPa, dual phase (DP) 590 MPa and transformation induced plasticity (TRIP) 590 and 780 MPa steels, all with a thickness of 2mm. Tensile samples were pre-strained, where possible, to elongations of 0%, 2%, 5%, 10%, 15%, 20% and 25%. These samples were then bake hardened using the conditions of 175°C for 30 minutes and subsequently strained till failure. The tensile curves are reported and the change in key deformation parameters with pre-strain and aging is discussed. The flow curves are used to derive more accurate flow stress models. The inclusion of these models in crash simulations will lead to better predictions and consequently to more appropriate materials selection.

9:45 AM

Deformation and Work Hardening of Cold Formed High Strength Steels at High Rates of Strain: *Taina Vuoristo*[1]; Veli-Tapani Kuokkala[1]; Marian Apostol[1]; Pasi Peura[2]; Juha Tulonen[2]; Janne Pirttijoki[2]; [1]Tampere University of Technology, Inst. of Matls. Sci., POB 589, Tampere 33101 Finland; [2]Rautaruukki Oyj, Harvialantie 420, Hämeenlinna 13300 Finland

Split Hopkinson Pressure Bar technique was used to study the high strain rate compression behavior of high and ultra high strength steel strips and tubes, including HSLA, dual-phase, and TRIP steels. In addition to the effect of loading rate, the effect of prior cold working on the high strain rate behavior of selected steels was studied. To obtain the desired strain rates for the thin sheet materials, a special stacking technique of specimens was successfully applied. The results assist the designer to choose advanced steels for structural parts subjected to various mechanical events, such as a car crash.

10:10 AM Break

10:25 AM

Recently Developed Testing Techniques and Dynamic Tensile Properties of Steel Sheets for Automobiles: *Shinji Tanimura*[1]; Masaki Uemura[2]; Nobusato Kojima[3]; Terumi Yamamoto[1]; [1]Aichi University of Technology, Dept. of Mech. Sys. Engrg., Gamagori-city, Aichi 443-0047 Japan; [2]Saginomiya Seisakusho, Inc., 535, Sasai, Sayama City, Saitama 350-1395 Japan; [3]Sumitomo Metal Industries Ltd., Corp. R&D Labs., 1-8 Fuso-cho, Amagasaki 660-0891 Japan

In order to analyze the dynamic behavior of parts of an automobile during a crash with sufficient accuracy, it is important to use a practical constitutive model that simulates the dynamic properties of the material of which the parts are composed. The model should be appropriate for a wide strain-rate range and a wide strain range, both of which are expected to occur during a crash. To establish the model, it is essential to study the dynamic properties of these materials over a wide strain-rate range and strain range. A brief review of principal features of the recently developed testing techniques based on the Sensing Block Method, which enables to obtain the entire tensile stress-strain curves for a wide strain-rate range on the order of 10-3 ~ 103 s-1 is presented. Application of the Sensing Block Method to dynamic buckling test and the dynamic response studies of parts are discussed. Recent studies on the required specimen geometry to accurately obtain the dynamic stress-strain curves for a wide strain-rate range[1] are also introduced and discussed. The entire tensile stress-strain curves of cold-rolled mild steel sheet (SPCE) and high strength steel sheets (SPFC440 and SPFC590), which are widely used for automobile structures, were obtained for a wide strain- rate range on the order of 10-3~103 s-1 by using the Sensing Block Type High Speed Material Testing System(Saginomiya,[2]). Based on an investigation of experimental data, strain rate sensitivities of flow stresses of these materials were clarified over a wide strain-rate range and strain range. The values of the true fracture strength and the true fracture strain were obtained by measuring the cross-sectional area at the ruptured part of the test piece, before and after testing. It was found that the values of the true fracture strength and the true fracture strain are substantially not affected by the strain rate over a wide range, up to high values in the order of 103 s-1. [1]Tanimura S., Tatsumi Y., Umeda T. and Kitada A., "Specimen Size Suitable for Material Testing at Medium and High Strain Rates", Transactions of the JSME, 68(676)(2002), pp.1762-1774. (in Japanese). [2]S. Tanimura, K. Mimura, and T. Umeda: New testing techniques to obtain tensile stress-strain curves for a wide range of strain rates, J. Phys. IV France Vol.110, pp.385~390(2003).

10:50 AM

The Effects of Strain Rate on the Deformation Behavior of High Strength IF and Bake-Hardenable Sheet Steels for Automotive Applications: *Ryan S. Kircher*[1]; Amar K. De[1]; John G. Speer[1]; David K. Matlock[1]; [1]Colorado School of Mines, Advd. Steel Procg. & Products Rsch. Ctr., 15th & Illinois, Golden, CO 80401 USA

The effects of strain rate on the deformation behavior of high strength bake-hardenable (BH) and interstitial free (IF) steels were evaluated on samples in the as received condition and after a laboratory bake-hardening treatment (2% pre-strain in tension followed by baking for 30 minutes at 1770C (3500F)). Tension tests were conducted at strain rates ranging from quasi-static to 200s-1. At quasi-static strain rates, the prestrained and baked BH material exhibited an appreciable increase in yield strength, consistent with anticipated bake hardening response for the alloy. With an increase in strain rate, however, the effects of bake hardening diminished at the highest strain rate the baked material had approximately the same mechanical properties as observed prior to the laboratory bake-hardening treatment. The tensile data on the BH steel are compared to similar data obtained on the high strength IF steel, and results obtained from crush-tower tests.

11:15 AM

Characterization of Strain and Strain Rate Histories in High Strength Steel During Asymmetric Tube Crush: *Srdan Simunovic*[1]; J. Michael Starbuck[1]; David Meuleman[2]; Raymond Boeman[1]; Phani V.V. Nukala[1]; [1]Oak Ridge National Laboratory, PO Box 2008, MS-6164, Oak Ridge, TN USA; [2]General Motors Corp., Mfg. Tech. Productionizing, 2000 Centerpoint Pkwy., Pontiac, MI 48341 USA

Asymmetric crushing of circular tubes made of mild and High Strength Steel has been investigated using constant velocity loading on hydraulically-driven equipment. Tube crush experiments were conducted using velocities within the range of quasi-static to 4 m/s. The characteristics of the testing equipment, primarily its high stiffness and ability to maintain constant velocity during crush, provided a controlled environment for detailed investigation of strain rate effects on a structural level. Strain histories were measured using resistance strain gages. The gages were positioned to coincide with the locations at or near plastic folds. The spatial distribution of the strain was measured by using multiple strain gages oriented in axial and hoop directions of the tubes. Formation of plastic hinges, strain, and strain rate histories were compared to the computational models. For the crush velocities and experimental techniques considered, results show that strain rate magnitudes of the order of 10+2/s prevail. Research was sponsored by the U.S. Department of Energy, Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Transportation Technologies, Lightweight Materials Program, under contract DE-AC05-00OR22725 with UT-Battelle, LLC. The support of Auto/Steel Partnership Strain Rate Characterization Team is acknowledged.

11:40 AM

Material Properties Considering Strain Rate Effect - Test Data Processing: *Wayne Li*[1]; Tau Tyan[1]; Yijung Chen[1]; Tsukasa Itoh[2]; [1]Ford Motor Co., EVB, MD 17, Rm. A100, 21500 Oakwood Blvd., Dearborn, MI 48121 USA; [2]Mazda Motor Corporation

Computer simulations have been utilized to study vehicle's crash responses during a high-speed impact condition. Studies conducted to improve vehicle's pulse prediction identified strain rate as one of the most critical factors in the modeling of vehicle components. Therefore, the strain rate effect needs to be taken into account in CAE simulation to accurately predict the different components' crash responses. In a study conducted by Volvo Car Corporation, the test data of 11 steels at different stain rates have been obtained and recommended for Radioss material law 36 input decks. The tabulated material law makes it possible to describe materials with different stress-strain curve patterns, convergent, parallel, or divergent. To accurately and efficiently create material input decks with strain rate consideration, a technique was developed to process and regularize strain rate test data. Previous investigation at Ford applied the technique to process the 11 strain rate test data. The regularized strain rate models were then applied to different vehicle models and satisfactory results were obtained. Since the many different steels are used in different vehicle programs, it is necessary to create the strain rate data that are not covered by the 11 steel data. More strain rate data obtained from tests will make it easier to incorporate strain rate effect in crash simulation that is intended to predict the behaviors of many different steels. In this study, strain rate test data provided by Mazda Motor Corporation for five steels are processed for Radioss material law 36 cards to expand the strain rate database for the crash CAE applications. These five materials are C14T, C16T, 6C59R, 6C78R, and SPCN2. The material input decks with strain rate consideration created in this study could be utilized directly in vehicle safety simulation to save time needed to process strain rate test data and minimize the error in preparing material input decks. The technique used to process and regularize the provided strain rate data is presented in this paper.

12:05 PM

Initial Chip Formation of Structural Steels Caused by Very High Strain Rates During Micro-Machining Processes: *Grant Mark Robinson*[1]; Mark James Jackson[1]; Luke Hyde[1]; [1]Tennessee Technological University, Ctr. for Mfg. Rsch., 115 W. 10th St., Brown Hall Rm. 222, Cookeville, TN 38505 USA

As micro and nanotechnology become increasingly important the need to create devices in engineering materials is more apparent. High-speed milling has proven successful at creating structures and texturing surfaces, especially in structural steels. Current cutting tools rotate around 250,000rpm; rotating the tool this quickly reduces cutting forces, which produces a higher quality of cut thus eliminating post processing. Clearly, strain rates imparted to the workpiece at these speeds are very high and this influences chip formation and chip removal mechanisms. High strain rates imparted cause distinct chip formations to occur which are also observed in other materials, most notably cancellous bone. Ductile materials such as aluminum do not machine well because they adhere to the cutting tool. This paper examines high strain rate initial chip formation in structural steel and compares these results to other materials.

Intellectual Property Fundamentals for Materials Scientists and Managers: IP Fundamentals I: Obtaining IP Rights

Sponsored by: TMS
Program Organizer: Steven P. Marsh, Frommer Lawrence & Haug LLP, New York, NY 10151 USA

Tuesday AM September 28, 2004 — Room: Grand Ballroom I — Location: Marriott New Orleans Hotel

Session Chairs: Steven P. Marsh, Frommer Lawrence & Haug LLP, New York, NY 10151 USA; Edgar H. Haug, Frommer Lawrence & Haug LLP, New York, NY 10151 USA; Grace L. Pan, Frommer Lawrence & Haug LLP, New York, NY 10151 USA

8:30 AM Invited
Intellectual Property: What Is It?: *Frommer Lawrence & Haug LLP*[1]; [1]745 Fifth Ave., New York, NY 10151 USA

Intellectual Property (IP) is a strange beast. The inventions, ideas, and goodwill that make up IP are treated in a legal sense like tangible property through the attachment of ownership rights. In broad terms IP can be divided into four main areas: Patents, which protect inventive devices and methods; Trademarks, which identify source of goods and provide “name brand” recognitions; Copyrights, which protect artistic and literary creations; and Trade Secrets, which are “private knowledge” that is kept secret from outsiders. Examples of each type of IP will be presented, with an emphasis on the structure of a patent and the rights afforded by it.

9:00 AM Invited
Overview of the U.S. Patent and Trademark Office: *Stephen G. Kunin*[1]; [1]U.S. Patent & Trademark Office, Commissioner for Patents, Washington, DC 20231 USA

Abstract not available.

9:30 AM Invited
Obtaining a Patent Through the United States Patent and Trademark Office: *Frommer Lawrence & Haug LLP*[1]; [1]745 Fifth Ave., New York, NY 10151 USA

Patents are granted by the United States Patent & Trademark Office (USPTO) through an application and review process. This process includes filing an application and supplemental document, and the “prosecution” phase of receiving and responding to Office Actions from the USPTO as necessary. An overview of the patent procurement process will be presented together with examples of typical fees and timetables.

10:00 AM Break

10:15 AM
A Tale of Two US Patents: *Krishnaswamy Sampath*[1]; [1]Consultant, 615 Demuth St., Johnstown, PA 15904 USA

Patents provide incentives to invent, invest in, and disclose new technology. By definition, an invention or discovery is something new and clearly distinguishable from prior art but is not a mere extension of prior art. Patents secure for limited times to inventors (or assignees) the exclusive right to their respective discoveries. This exclusive right precludes others from using the invention without an appropriate licensing agreement. An anomalous situation has occurred when the USPTO awarded two US Patents (5,523,540 and 5,744,782) to two different assignees for essentially the same product: gas metal arc welding electrodes for joining certain high strength steels (such as HY-80, HY-100, HY-130, HSLA-80 and HSLA-100) used in naval hull construction of both surface and stealth vessels. These welding electrodes resist hydrogen assisted cracking while welding, without a need for substantial preheating. This paper examines the technological tale of these two US patents.

10:30 AM Invited
Responding to the Inventors Muse: Personal Experiences in the Patent Arena: *Iver Eric Anderson*[1]; [1]Iowa State University, Ames Lab. (USDOE), Matls. & Engrg. Physics, 222 Metals Dvlp. Bldg., Ames, IA 50011 USA

Opportunities for invention often lie at the seams of technological disciplines. This talk will discuss personal case histories of discoveries that grew from interdisciplinary collaborations to solve persistent problems in materials science. Novel solutions typically arise from base knowledge in unrelated areas, are motivated by counteraction to accepted beliefs, and require a twist of inspiration. One critical element in a successful patent application is the ability of your patent attorney to grasp the essential technical aspects of your invention in order to properly “teach the art” in your patent. The patent path can lead to a long journey that requires persistence and patience to finally see your idea in the commercial marketplace. Common barriers to licensing and technology transfer normally will be encountered, but can be overcome with guidance from experts in the technology and intellectual property field. Support from Iowa State University Research Foundation and USDOE-BES (contract no. W-7405-Eng-82).

11:00 AM Invited
Obtaining Trademarks and Utilizing Them Effectively: *Anna Erenburg*[1]; [1]Gottlieb, Rackman & Reisman P.C., 270 Madison Ave., New York, NY 10016 USA

Trademarks often take a back seat to patents, but they can add significant value to patented technologies. This presentation will cover trademark basics, such as what a trademark is, how to obtain and maintain a trademark registration in U.S. and abroad, and the scope of protection afforded by a registration. Additionally, the presentation will discuss how trademarks can extend the commercial value of a patented technology beyond the lifetime of a patent. This presentation will include many visual examples and a selection of useful trademark information sources.

11:30 AM Invited
Protecting IP Assets Worldwide: *Norbert Hansen*[1]; Korbinian Kopf[1]; [1]Maiwald Patentanwalts GmbH, Elisenhof, Elisenstrasse 3, Munich, Bavaria 80335 Germany

Global business activities require more than local protection in your home country. A granted patent gives its owner an exclusive right to prevent competitors from using the invention protected. However, patent law is national law limiting the patent’s effects territorially, so if you intend to market your innovations internationally you have to seek for patent protection in several countries worldwide. There are many ways to obtain patent protection on an international basis. Based on your national filing, a patent application under the Patent Cooperation Treaty (PCT) provides a flexible and effective tool for applying for protection in more than 120 countries worldwide. The PCT system further offers an international search for prior art and an optional preliminary examination procedure, before deciding in which countries a national proceeding should be started. If Europe is the market, an application for the grant of a European patent gives you a patent in almost thirty member countries all over Europe in one single patent grant procedure. Since examination is rigorous under the European patent system, the outcome is a strong patent which is a valuable tool keeping competitors and product copyists from taking advantage from your research results. An overview will be given on the available international patent application systems, as well as an analysis of their advantages and drawbacks. International patent strategies will be presented to provide an overview on how IP rights may support your company’s global activities.

Materials Damage Prognosis: Multi-Scale Modeling and Simulation

Sponsored by: TMS - Structural Materials Division
Program Organizers: James M. Larsen, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson AFB, OH 45433-7817 USA; Jeffrey R. Calcaterra, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson Air Force Base, OH 45433-7817 USA; Leo Christodoulou, Defense Advanced Research Agency, Arlington, VA 22203-1714 USA; Michael L. Dent, Anteon Corporation USA; William J. Hardman, Naval Air Systems Command, Propulsion and Power Directorate (AIR 4.4.2), Patuxent River, MD 20670-1534 USA; Paul Hoffman, United States Navy, NAVAIR, Patuxent River, MD 20670 USA; J. Wayne Jones, University of Michigan, College of Engineering, Department of Materials, Science and Engineering, Ann Arbor, MI 48109 USA; Stephan M. Russ, Air Force Research Laboratory, Materials and Manufacturing Directorate, AFRL/MLLN, Wright-Patterson Air Force Base, OH 45433-7817 USA

Tuesday AM Room: La Galerie 6
September 28, 2004 Location: Marriott New Orleans Hotel

Session Chairs: J. Wayne Jones, University of Michigan, Matls. Sci. & Engrg., Ann Arbor, MI 48105 USA; Reji John, Air Force Research Laboratory, Wright Patterson AFB, OH 45433-7817 USA

8:30 AM Invited
Damage Detection and Prediction for Composite Plates: *Charles R. Farrar*[1]; Jeannette Wait[1]; Trevor B. Tippetts[1]; Francois M. Hemez[1]; Gyuhae Park[1]; Hoon Sohn[1]; [1]Los Alamos National Laboratory, MS T-006, Los Alamos, NM 87545 USA

This paper will summarize results from Los Alamos National Laboratory's (LANL) damage prognosis project that is studying projectile impact induced damage on composite plates. First, the experimental/analytical program will be summarized. More specifically, the advanced active sensing technologies being employed for this study along will be discussed along with newly developed data interrogation algorithms that will allow one to locate a delamination within the composite structure. This discussion will be followed by a summary of the numerical models that have been developed for damage initiation and evolution prediction and the validation studies that are being conducted to assess the predictive accuracy of these models. The presentation will conclude with an introduction to a joint research effort with the University of California, San-Diego that aims to transition this technology to actual unmanned aerial vehicles.

8:55 AM
Cumulative Damage Models for Single Crystal Nickel Based Superalloy Under Creep and Fatigue Loading: *Mandar Chati*[1]; Dana Swalla[1]; James Laflen[2]; [1]General Electric, Global Rsch. Ctr., Lifing Tech. Lab., One Rsch. Cir., Bldg. K1, 3A27A, Niskayuna, NY 12309 USA; [2]General Electric Transportation, 1 Neumann Way, Cincinnati, OH 45215 USA

A simplified approach to creep and fatigue damage prediction using a cumulative damage model is developed and applied for Rene N5, a single crystal nickel based superalloy material commonly used in aircraft engine turbine blades. Various cumulative damage models previously presented in the literature for this material are also presented for comparison. The procedures used to account for a number of mechanisms responsible for creep and fatigue damage are reviewed for each model. This cumulative damage approach has been used to predict failure for simple test cases. Several material tests on a tubular geometry (with holes) subjected to complex mission cycles are planned to validate the cumulative damage model approach.

9:20 AM
Deterministic Modeling of Alloy 22 Uniform Corrosion: Model Parameter Derivation from Electrochemical Impedance Spectroscopy Data: *L. Glen McMillion*[1]; Adan Sun[2]; Digby D. MacDonald[3]; Shantanu A. Namjoshi[1]; [1]University of Nevada, Metallurgl. & Matls. Sci. Engrg., Coll. of Engrg., MS 388, Reno, NV 89557 USA; [2]Pennsylvania State University, Matls. Sci. & Engrg., 31 Hosler Bldg., Univ. Park, PA 16802 USA; [3]Pennsylvania State University, Matls. Sci. & Engrg., 0201 Steidle Bldg., Univ. Park, PA 16802 USA

Uniform corrosion of Alloy 22 is difficult to measure by conventional weight loss methods because the times required to sustain measurable damage are prohibitive. Therefore deterministic models that rely upon time-invariant physical laws are necessary to predict corrosion damage. The Point Defect Model (PDM) of passive film growth and breakdown on alloys in aqueous solutions is such a model. Model parameters, including rate constants for the fundamental reactions of the passive film, must be determined from experimental data. Electrochemical Impedance Spectroscopy (EIS) data were measured for Alloy 22 potentiostatically over the passive potential range in deaerated solutions of 0.1 M NaCl at 30°, 60°, and 90°C, and pH 3 and 11. Optimization of the PDM on the impedance data has yielded parameters for predicting uniform corrosion damage for Alloy 22. These PDM parameters may be combined with a pit growth model to develop damage functions for localized corrosion.

9:45 AM
Prediction of Scatter in Fatigue Properties Using Discrete Damage Mechanics: Antonio Rinaldi[1]; *Pedro Peralta*[1]; Dusan Krajcinovic[1]; [1]Arizona State University, Mechl. & Aeros. Engrg., Tempe, AZ 85287-6106 USA

Discrete damage mechanics has been used to simulate the fatigue scatter in a generic metallic material using a 2-D disordered lattice model, where the nodes of the network represent individual grains and the axial elements represent grain boundaries. Geometrical disorder was introduced by creating a non-periodic, irregular Delaunay network topology. The static strength of the elements followed a normal distribution and their fatigue behavior was represented by a Basquin-type equation. Damage accumulation was assumed to follow the Palgrem-Miner rule. The lattice was cycled under total strain control and at least 100 simulations were performed at each strain amplitude to gather statistics. It was found that this relatively simple model predicts a macroscopic Coffin-Manson behavior and that the fatigue life at a constant strain follows a log-normal distribution, which allows to predict fatigue properties at different probabilities of failure. Extension and calibration of this model for actual materials will be discussed.

10:10 AM Break

10:20 AM Invited
Simulation of Fatigue Crack Initiation in Aluminum Alloys Using Realistic Microstructures: *Anthony R. Ingraffea*[1]; A. Maniatty[2]; A. D. Rollett[3]; [1]Cornell University, Ithaca, NY 14853 USA; [2]Rensselaer Polytechnic Institute, Troy, NY 12180 USA; [3]Carnegie Mellon University, Pittsburgh, PA 15213 USA

We are developing physics-based models for simulating initiation of fatigue cracks in aluminum alloys. Our models are part of a large, DARPA-funded project on structural integrity prognosis. The salient features of our approach are: The use of statistically representative, realistic microstructures as a starting point for our simulations. Using unique microstructure builder tools, we assemble three-dimensional digital material representations from actual microstructural observations. These contain realistic textures, particle distributions, etc. Constituents are assigned statistically representative distributions of properties such as yield strengths and toughnesses. The use of polycrystal plasticity models to accurately compute stress and strain fields in polycrystals using the finite element method. In polycrystalline metals, the grain structure and phenomena occurring on the grain scale, such as interactions between grains and particles and crystallographic slip, strongly influence the fatigue behavior of the materials. Statistically realistic 3D microstructures are directly simulated in order to investigate the effect of elasto-plastic response within the microstructure on the fatigue behavior. Different slip system hardening models are considered and the influence of self vs. latent hardening is investigated. The influence of slip system hardening vs. geometric effects associated with the microstructure and grain orientations are also being studied. The use of explicit geometric representations of fatigue-crack precursors in a finite element model, such as grain boundaries or particle decohesion, and to allow these to evolve through changes in the underlying geometric and mesh models though the course of a simulation. The use of multi-scale finite element modeling to incorporate the effect of microstructure scale damage nucleation and evolution on the predictions of fatigue life for vehicle scale components. We will report on progress in development, verification, and validation of our simulation models, and show example simulations on test specimens and actual flight components.

10:45 AM
3D Microstructures for Prognosis Modeling: *Anthony D. Rollett*[1]; Abhijit Brahme[1]; Joseph Fridy[2]; Sukbin Lee[1]; David Saylor[3]; [1]Carnegie Mellon University, Matls. Sci. & Engrg., 5000 Forbes Av., Pittsburgh, PA 15213 USA; [2]Alcoa, Techl. Ctr, 100 Techl. Dr., Alcoa Ctr., PA 15069 USA; [3]U.S.F.D.A., 12725 Twinbrook Pkwy., Rockville, MD 20852 USA

An essential element of connecting microstructure to damage accumulation via simulation is to be able to construct sufficiently accurate descriptions of a material in all three dimensions. The Microstructure Builder provides a set of tools for accomplishing this. Automated electron backscatter diffraction based on scanning electron microscopy is used to characterize at least two different mutually perpendicular cross-sections. The resulting orientation and misorientation distribution information, together with size and aspect ratio distributions are used to generate the microstruc-

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tures. The grain geometry is discretized with a Voronoi tessellation which can be subsequently converted to a finite element mesh. Groups of cells are aggregated to form grains and orientations are assigned using a simulated annealing procedure to match the experimentally measured distributions. This description of a single-phase material has been extended in this work to describe materials such as aerospace aluminum alloys that are essentially single phase but have coarse inclusions. The dispersion of second phase particles is fit using anisotropic pair correlation functions. The microstructures thus generated will be used to study the effect of features such as second phase particles and triple junctions on fatigue crack initiation.

11:10 AM Invited
Fretting Fatigue of Ti-6Al-4V: A Micromechanical Approach: Jason Mayeur[1]; Richard W. Neu[1]; *David L. McDowell*[1]; [1]Georgia Institute of Technology, GWW Sch. of Mechl. Engrg., Atlanta, GA 30332-0405 USA

Both 2-D and 3-D crystal plasticity models are developed for dual-phase Ti-6Al-4V and used to investigate and quantify the influence of microstructural heterogeneity on cyclic microplastic deformation and cumulative ratchet strain for representative fretting contact conditions. Fretting experiments, which involve reciprocating sliding of a cylindrical body over a flat body at small relative slip amplitudes, indicate that crack formation in the surface layers is affected by a plastic ratcheting mechanism. In an aerospace gas turbine engine, the dovetail joint between the blade and disk is prone to fretting. It is useful to examine the fretting fatigue problem using microstructurally-based models given that the length scales at which fretting fatigue cracks initiate are on the order of microstructural dimensions and initiation sites are likely to be influenced by the highly heterogeneous nature of these materials at this scale. Fretting simulations using a simplified 2-D planar triple slip crystal plasticity model, compared to simulations conducted using a conventional J2 initially homogeneous plasticity model with non-linear kinematic hardening, indicate that crystal plasticity is necessary to capture the shear localization and dominant plastic ratchetting deformation mechanism in the near surface layers and hence provides much more realism in problems dealing with plastic deformation at fretting and sliding contacts. Idealized fretting contacts are analyzed to construct fretting maps that may be useful in design. The constitutive model is extended to 3-D and applied to behavior of an equiaxed duplex microstructure of Ti-6Al-4V consisting of primary-nalpha-phase grains and secondary alpha + beta lamellar grains. The primary alpha-phase is of hcp crystal structure and the alpha + beta lamellar grains consist of alternating plate-like layers of a secondary alpha-phase and a bcc beta-phase, which are subject to a burgers orientation relation. We explore implications of slip system anisotropy, incompatibility at grain and phase boundaries, microtexture, and phase distribution in relation to the plastic strain evolution during the fretting process.

11:35 AM Invited
Physics-Based Modeling of Composite Materials: *Todd O. Williams*[1]; Trevor B. Tippetts[1]; [1]Los Alamos National Laboratory, Los Alamos, NM 87545 USA

This presentation will discuss the physics-based modeling component of a damage prognosis effort at Los Alamos National Laboratory. The particular problem being considered is the prediction of the behavior, including damage initiation and evolution, of a moderately thick, quasi-isotropic Gr/Ep composite plate subjected to impact and subsequent fatigue loading. The modeling effort for this project is proceeding along three different length scales, the macroscopic, the mesoscopic, and the microscopic. A novel general, multilength scale plate theory (GMLSPT) and its associated finite element implementation are being used to model all aspects of the behavior of the entire plate and the individual lamina within the plate. This theory considers fracture in the form of delamination between plies as well as ply splitting through the use of cohesive zone models (CZM) and a robust adaptive integration scheme. A nonlinear CZM and a bilinear CZM are currently being utilized in the GMLSPT analysis. An adaptive integration scheme is necessary to allow the efficient analysis of large-scale structures. A novel stochastic micromechanical theory has been developed to model the material behavior at the lamina level. This micromechanical theory incorporates probability distribution functions (PDFs) for how the applied bulk fields drive both elastic and inelastic localization processes within the composite microstructure. In the current work, the inelastic localization phenomena consider both time dependent deformations (such as viscoelasticity) as well as damaging mechanisms. The use of PDFs for the localization effects allows the efficient analysis of both the inelastic deformation of heterogeneous materials as well as their fracture behavior. The abilities of the proposed hierarchical modeling framework to accurately predict damage accumulation over varying time and length scales are illustrated through different examples based on comparisons with both analytical results and experimental results.

Modeling and Computer Applications in Metal Casting, Shaping & Forming Processes: Modeling and Computer Simulation: Thermal Treatment and Related Processes

Sponsored by: AIST, TMS - Extraction & Processing Division, TMS - Materials Processing & Manufacturing Division, TMS, TMS - MPMD/EPD-Process Modeling Analysis & Control Committee, TMS - MPMD-Shaping and Forming Committee, TMS - MPMD-Solidification Committee, AIST - Division VI, AIST - Division VII, TMS - MPMD-Computational Materials Science & Engineering-(Jt. ASM-MSCTS)
Program Organizers: Krich Sawamiphakdi, The Timken Company, R&D Manufacturing Technology, Canton, OH 44706 USA; Praveen Pauskar, The Timken Company, Advanced Process Technology, Timken Research, Canton, OH USA; Maciej Pietrzyk, Akademia Gorniczo-Hutnicza, Department of Computer Methods in Metallurgy, Krakow Poland; Raghavan Srinivasan, Wright State University, Department of Mechanical & Materials Engineering, Dayton, OH 45435 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA; Brian G. Thomas, University of Illinois, Department of Mechanical and Industrial Engineering, Urbana, IL 61801 USA

Tuesday AM	Room: La Galerie 2
September 28, 2004	Location: Marriott New Orleans Hotel

Session Chairs: Krich Sawamiphakdi, The Timken Company, Advd. Process Tech., Canton, OH 44706-0930 USA; Calvin T. Tszeng, Illinois Institute of Technology, Dept. of Mechl. Matls. & Aeros. Engrg., Chicago, IL 60616 USA

8:30 AM
Data Needs for Modeling Heat Treatment of Steel Parts: *B. Lynn Ferguson*[1]; Zhichao Li[1]; Andrew M. Freborg[1]; [1]Deformation Control Technology, Inc., 7261 Engle Rd., Ste. 105, Cleveland, OH 44130 USA

Hardening of steel parts involves controlling the microstructural phases by heating and cooling at particular rates and holding times. The microstructure changes from an initial form that is typically ferrite and pearlite, to austenite at high temperatures, and to combinations of martensite, bainite, pearlite and ferrite upon quenching and tempering. There is associated thermal expansion/contraction of these phases, changes in density as phases transform, and resultant stress that accompanies both nonuniform heating/cooling and the changes in phase. Simulation requires that the material behavior be defined for all possible conditions experienced during heat treatment. Carburization or another surface chemistry modification adds to the complexity because the mechanical, thermal and metallurgical properties change with chemistry, especially carbon content. This talk discusses the nature of the data required to characterize steels for heat treatment, and presents some methods for checking data accuracy and material response to heat treating processes.

8:55 AM
Improving the Bend Fatigue Strength of Carburized Gears: *B. Lynn Ferguson*[1]; Andrew M. Freborg[1]; David Schwam[2]; [1]Deformation Control Technology, Inc., 7261 Engle Rd., Ste. 105, Cleveland, OH 44130 USA; [2]Case Western Reserve University, Matls. Sci. & Engrg., 10900 Euclid Ave., Cleveland, OH 44106 USA

An objective of the Army ATD is to improve the power density and life of helicopter transmissions. If the fatigue lives of current gears can be improved by a standard manufacturing process such as heat treatment, costly redesign can be avoided. This paper discusses a Phase I SBIR project with a goal of a 25% improvement in the bending fatigue life of carburized Pyrowear 53 steel gears. This effort was a combination of simulation and experiments, with the quenching process being a primary variable being examined to achieve the project goal. DANTE heat treat simulation software was used to predict residual stress levels for oil and intensive quenching processes. Test pieces were machined and heat treated, and then tested using three point bending to simulate cyclic stresses in the root of a gear. This paper presents simulation results and bending fatigue test data.

9:20 AM
Modeling the Austenite Decomposition During Continuous Cooling: *Gonzalo Roberto Gomez*[1]; Martin Bühler[1]; Teresa Perez[1]; [1]CINI-FUDETEC, Dept. de Metalurgia, Dr. Simini 250, Campana, Buenos Aires 2804 Argentina

A metallurgical model to describe the formation of ferrite, perlite and bainite during continuous cooling was developed. The model uses the classical nucleation theory to calculate the beginning of the reaction, and Avrami-type equations to evaluate the transformation progress. The materials studied were plain carbon and microalloyed steels with Nb, Ti and/or

V additions. The predictions of transformation kinetics, final phase distributions and ferritic grain sizes were compared to experimental results obtained from continuous cooling tests performed at a thermo-mechanical simulator (cooling rates between 1°C/sec and 50°C/sec).

9:45 AM Break

9:55 AM
A Technique to Extract Overall Kinetics of Metallurgical Changes From Macroscopic Behavior: *T. C. Tszeng*[1]; [1]Illinois Institute of Technology, Thermal Procg. Tech. Ctr., Dept. of Mechl., Matls. & Aeros. Engrg., Chicago, IL 60616 USA

This paper presents the development of an algorithm that is able to accurately identify the overall kinetics of metallurgical changes from macroscopic behavior. Such algorithm is useful in the computational study as well as practical design of more efficient manufacturing processes in metals processing. Specifically, the fundamental parameters governing the nucleation and growth of the metallurgical features by diffusional transformations are determined by minimizing the error between the measured macroscopic behavior (e.g., dilatometry) and that calculated by the prespecified kinetic model. In the process, the progress of metallurgical transformation in the particular tests can also be determined simultaneously. The accuracy and applicability of the developed algorithm is demonstrated by using the dilatometry data of AISI 1080 steel in austenitization as well as several hypothetical transformations.

10:20 AM
Computer Simulation of High Pressure Gas Quenching Process: *Mohammed Maniruzzaman*[1]; Michael B. Stratton[1]; Richard D. Sisson[1]; [1]Worcester Polytechnic Institute, Matls. Sci. & Engrg., Mechl. Engrg. Dept., 100 Inst. Rd., Worcester, MA 01609 USA

With increasing pressure capabilities of gas quenching vacuum furnace, gas quenching is becoming a viable alternative of liquid immersion quenching of steel. Gas composition, pressure and gas circulation velocity are three important parameters that control the heat extraction rate from the quenched part surface. Computational fluid dynamics simulation is used to compute the surface heat transfer coefficients as a function of temperature at different pressure and gas velocity level for nitrogen gas. The results are the input as a process variable to a Finite Element based heat treatment simulation software to predict the metallurgical phase distributions, residual stress distributions and the dimensional stability of the quenched parts. Several numerical experiments are performed to predict the effects of the gas pressure and the gas velocity on these physical and microstructural parameters.

10:45 AM
Effect of Non-Uniform Surface Heat Extraction on Dimensional Stability of a Quenched Part: *Mohammed Maniruzzaman*[1]; Jiankun Yuan[1]; Richard D. Sisson[1]; [1]Worcester Polytechnic Institute, Matls. Sci. & Engrg., Mechl. Engrg. Dept., 100 Inst. Rd., Worcester, MA 01609 USA

Distortion and cracking of a metallic part quenched in a quenchant can be reduced greatly by improving quench uniformity. In this study, numerical experiments are performed to investigate the sensitivity of heat treatment response to non-uniformity of heat extraction rate of a steel plate quenched in liquid quenchant. The surface heat transfer coefficient (h) as a function of temperature is the input as a process variable to heat treatment simulation software DANTE/ABAQUS to predict the residual stress state and distortion of the plate. The results are analyzed as a ratio of h for front face to h for back face of the plate to determine the optimum h ratio for minimum distortion.

11:10 AM
Production of Nanocrystalline Aluminium by ECAP of Cylindrical Billets: *Andrzej Rosochowski*[1]; Lech Olejnik[2]; Maria Richert[3]; [1]University of Strathclyde, Design, Manufacture & Engrg. Mgmt., James Weir Bldg., 75 Montrose St., Glasgow G1 1XJ UK; [2]Warsaw University of Technology, Matls. Procg., Narbutta 85, Warsaw 02-524 Poland; [3]University of Mining and Metallurgy, Non-Ferrous Metals, Mickiewicza 30, Cracow 30-059 Poland

Nanometals (metals with ultra fine grain structure) produced by severe plastic deformation (SPD) possess a range of unique mechanical and physical properties such as exceptional strength with good ductility, high hardness, high low-temperature impact strength as well as improved fatigue life, diffusivity, magnetic properties, resistance to friction, resistance to thermal erosion, etc. Possible applications are wide ranging including: materials for MEMS, aerospace, automotive, defence, medical and sports industries. The proposed paper introduces a new SPD process based on equal channel angular pressing of cylindrical billets. The material flow in the process is simulated using a Finite Element Method (FEM) and a classical strain-hardening model. Using appropriate tooling, ECAP trials of 99.6% pure aluminium are carried out. The resulting microstructure and tensile properties of the processed material are discussed. The anomalous yield behaviour of the nanomaterial is also analysed with a view to using it in future FEM simulations.

11:35 AM
Development of Dislocation Model with Recrystallization and Parameters Evaluation by the Methods of Control Theory: *Dmitry S. Svyetlichnyy*[1]; Henryk Dyja[1]; [1]Czestochowa University of Technology, Faculty of Process & Matls. Engrg. & Applied Physics, Al. Armii Krajowej 19, Czêstochowa 42-200 Poland

A model of flow stress with recrystallization based on the dislocation theory is presented in the paper. The model developed by using the approaches of control theory allows for prediction of dislocation density not only during the deformation, but also in the pauses between the deformations. Model's parameters are defined by comparison of the calculated curve with the measured flow stress curve. The integral quadratic criterion is applied to modeling of data. Integral dependences of the dislocation model leads to the using of the integration of ordinary differential equations and non-gradient methods of minimization. If the differential equations described dislocation evolution are considered as a state-space model, methods of solution this optimal control problem could be straight used. In the paper presented solution algorithm and an example of parameters calculations.

12:00 PM
Multi-Scale Characterization of Shear Localization in Continuous Cast Automotive Sheet AA5754: *J. Kang*[1]; M. Jain[2]; D. S. Wilkinson[1]; J. D. Embury[1]; [1]McMaster University, Dept. of Matls. Sci. & Engrg., Hamilton, Ontario L8S 1J4 Canada; [2]McMaster University, Dept. of Mechl. Engrg., Hamilton, Ontario L8S 1J4 Canada

Multi-scale characterization of shear localization in continuous cast AA5754 aluminum alloy sheet is presented in the present study. Strain mapping has been conducted at two levels. Full-field strain mapping based on digital speckle correlation method was used to explore the macroscopic shear localization process. The results show that the shear localization emerged after type-B Portevin-Le Chatellier bands during deformation. Eventually one of these PLC bands interacts with the shear bands and leads to the final localized necking and failure of the material. In addition in-situ uniaxial tensile tests were conducted in a field-emission scanning electron microscope (FE-SEM) to reveal that slip lines developed during deformation. By utilizing the SEM topography correlation method, full-field strain mapping at grain level is realized. The results show that local strain at grain level can reach the order of 1 and reveal how slip between grains becomes connected. Based on the above observations, the sequences of the events in the development of tensile instability of continuous cast automotive sheet AA5754 are discussed and clarified.

Pb-Free and Pb-Bearing Solders: Session III

Sponsored by: TMS - Electronic, Magnetic & Photonic Materials Division, TMS - EMPMD-Electronic Packaging and Interconnection Materials Committee
Program Organizers: C. Robert Kao, National Central University, Department of Chemical and Materials Engineering, Chungli City 32054 Taiwan; W. Plumbridge, Open University, School of Engineering Materials, Milton Keynes MK7 6AA UK; K. N. Subramanian, Michigan State University, Chemical Engineering & Material Science, East Lansing, MI 48824 USA

Tuesday AM — Room: Grand Ballroom K
September 28, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: K. N. Tu, University of California, Dept. of Matls. Sci. & Engrg., Los Angeles, CA 90095 USA; C. R. Kao, National Central University, Dept. of Chem. & Matls. Engrg., Chungli City Taiwan

8:30 AM Invited
Mechanism of Spontaneous Sn Whisker Growth: *K. N. Tu*[1]; [1]University of California, Dept. of Matls. Sci. & Engrg., Los Angeles, CA 90095-1505 USA

Leadframes used in surface mount packaging technology were finished with a layer of Pb-free solder for passivation and enhancing solder wetting. On the surface of eutectic SnCu finish, a large number of Sn whiskers are found to grow at room temperature The long ones can become shorts between the neighboring legs of the leadframe. In this talk, structure and stress analyses by using micro x-ray-diffraction in synchrotron radiation will be reported. Cross-sectional scanning and transmission electron microscopy will be presented with samples prepared by focused ion beam. The mechanism of spontaneous Sn whisker growth will be analyzed; both room temperature Cu-Sn reaction and protective surface

Sn oxide are found to be necessary conditions for the whisker growth. How to suppress and how to accelerate Sn whisker growth will be discussed.

9:00 AM Invited
Synchrotron X-Ray Microdiffraction Analysis of Whisker Growth in Sn Films: *Wenjun Liu*[1]; Gene Ice[1]; Ben Larson[1]; Peter J. Bush[2]; [1]Oak Ridge National Laboratory, UNICAT, Advd. Photon Source, 9700 S. Cass Ave., Argonne, IL 60439 USA; [2]State University of New York, Buffalo, NY 14214 USA

Whisker growth in Sn films is an example of anomalous grain growth and an area of long-standing interest to the application of Pb-free solder in electronic manufacturing. Possible mechanisms of whisker development include special grain orientations, grain boundaries, local residual stresses, or combinations of these factors. Recent measurements on the UNICAT beamline at the Advanced Photon Source (APS) illustrated the ability of a newly developed three-dimensional polychromatic x-ray microscope to characterize the local orientation and strain of whiskers and near whisker regions. With unprecedented special resolution of approximately 0.5 x 0.5 x 1.0 um3 and angular resolution of 10-4, the local grain orientation, grain boundary types, as well as the elastic and plastic deformation, will provide for a powerful test of whisker growth theories. Research supported by the DOE, Division of Materials Sciences under contract with ORNL, operated by UT-Battelle, LLC. UNICAT is supported by ORNL, UIUC-MRL, NIST, and UOP Inc.

9:30 AM
Analysis Pb-Free Solders Using Synchrotron X-Ray Diffraction Techniques: *Chris John Bailey*[1]; [1]University of Greenwich, Sch. of Computing & Math. Scis., Old Royal Naval College, Maritime Greenwich, Greenwich, London SE10 9LS England

The intense flux of high-energy X-rays provided by synchrotron radiation sources allows transmission diffraction experiments to be performed. This can be used to gain non-destructive phase and strain data from the bulk of solid materials. The ability to focus the beam of x-rays into a narrow beam or spot of monochromatic x-rays allows 2d and even 3d mapping to be performed. This paper will show results from experiments undertaken at the European Synchrotron Radiation Facility. In these experiments, lead-free solder joints were examined and the data gathered analysed to identify the microstructure in the joints of different ages. Samples of solder paste were also analysed during thier melting and solidification. Time-resolved x-ray diffraction data were collected both from the bulk solder and interfacial regions during this melting and solidification processes. The paper will discuss the formation of microstructure for different pad finishes and cooling rates.

9:55 AM
Assessment of Internal Damage Accumulation from Thermal Excursions in Sn-Based Solder Joints: J. G. Lee[1]; K. N. Subramanian[1]; *A. Lee*[1]; E. D. Case[1]; T. Hogan[2]; [1]Michigan State University, Dept. of Chem. Engrg. & Matls. Sci., E. Lansing, MI 48824-1226 USA; [2]Michigan State University, Dept. of Elect. & Computer Engrg., E. Lansing, MI 48824-1226 USA

Damage resulting from thermal excursions in Sn-based solder joints builds up internally without any surface manifestations until very late in service life. As a consequence surface characterization of the solder joints will not be presenting the true picture of the damage accumulation that controls the reliability of the joint. Sectioning to study such internal damage accumulation will alter the true features of the damage in the soft solder material resulting in false interpretations. In addition, such sectioning will destroy the specimen with no possibility to follow the progress of damage during further thermal exposures. Preliminary results obtained with non-destructive evaluation methods employed to assess the internal damage build-up from thermal excursions in Sn-based solder joints will be presented. Work supported by the National Science Foundation under grant NSF DMR-0081796 and NSF DMI-0339898.

10:20 AM Break

10:35 AM
The Study of Microstructure Evolution of Tin Grains Due to Electromigration by Using Synchrotron Radiation: *Albert T. Wu*[1]; KingNing Tu[1]; [1]University of California, Matls. Sci. & Engrg., 1677 Boelter Hall, Los Angeles, CA 90095 USA

White â-Sn has a body-center tetragonal (BCT) structure. Under electromigration, pure Sn stripe shows an unexpected voltage drop about 10%. The resistivity of a, b axes are 65% smaller than that of c axis. It is believed that the drop on voltage is contributed to the anisotropic property, hence causes microstructure evolution under current stressed. Synchrotron radiation is a unique apparatus since it provides small beam (~1µm), which is comparable to the grain size. We are able to do grain-by-grain analysis on the changes of grain orientation before and after electromigration by analyzing diffraction Laue Pattern. We observe high resistance grains rotate and re-oriente to the low resistivity direction.

11:00 AM
Ultra Fast Cu Disslolution Induced by Electric Current in Flip Chip Solder Joints: C. M. Tsai[1]; Y. C. Hu[1]; *C. Robert Kao*[1]; [1]National Central University, Dept. of Chem. & Matls. Engrg., Chungli City 320 Taiwan

A new electromigration failure mechanism in flip chip solder joints is reported. The solder joints failed through a very rapid, localized dissolution of the Cu on the cathode side. The regions of the dissolved Cu include not only the Cu under bump metallurgy but also the internal Cu conducting trace on the chip. From the location and geometry of the dissolved Cu, it can be concluded that current crowding played an important role for the rapid dissolution. The dissolved Cu atoms were then driven by electrons to the anode side, and a large amount of Cu6Sn5 was formed there. To avoid this type of failure, another metal more resistant to dissolution should be used in place of or over Cu. Moreover, the geometry of the under bump metallurgy and conducting trace might have to be carefully designed to achieve a more uniform current distribution to reduce the effect of current crowding.

11:25 AM
Polarity Effect of Electromigration on Intermetallic Compound Growth in Lead-Free Solder Lines: *Shengquan Ou*[1]; Hua Gan[1]; King-Ning Tu[1]; [1]University of California, Matls. Sci. & Engrg., 405 Hilgard Ave., Los Angeles, CA 90095-1595 USA

Electromigration has become a reliability problem in flip chip solder joints. To study the problem, we have prepared test samples of Pb-free solder lines in v-grooves etched on (001) Si wafer surfaces. The advantages of using v-groove samples are that we can apply a rather high current density and there is no current crowding. Stressing at 1×104 A/cm2 to 4×104 A/cm2 at 150°C, we observed polarity effects of electromigration on intermetallic compound (IMC) growth at the Ni (or Cu) cathode and anode; the growth is faster at the anode. Kinetic measurement and analysis of IMC growth in eutectic SnAg and SnAgCu v-groove solder lines with Ni (or Cu) electrodes have been carried out. The polarity effect of interaction between chemical and electrical driving forces on IMC growth will be discussed.

11:50 AM
Electromigration in Eutectic SnPb Solder Strips: *Chung-Kuang Chou*[1]; Yin-Ting Yeh[1]; Chih Chen[1]; [1]National Chiao Tung University, Dept. of Matl. Sci. & Engrg., 1001 Ta-hseuh Rd., Hsin-chu 30050 Taiwan

Electromigration emerges to be an important reliability issue in microelectronic packaging industry as the dimension of solder joints keeps shrinking. However, the important electromigration parameters of in the eutectic solder is still unknown. In this study, eutectic SnPb solder was reflowed on patterned 0.4 µm Cu/ 0.15 µm Ti films to fabricate solder Blech (strips) structure. Then the solder was polished to obtain a smooth surface, and the final thickness of the solder is about 3 µm. The advantage of this structure is that depletion volume of solder due to electromigration can be measured preciously. Atomic Force Microscope (AFM) was employed to measure the depletion volume near the cathode end. Then electromigration rate at various current densities and temperatures can be measured. The important electromigration parameters, such as electromigration rate, threshold current density, effective charge numbers, and activation energy will be presented in the conference.

Precipitation in Steels - Physical Metallurgy and Property Development: HSLA Steels: Cu-, Cr-Precipitation

Sponsored by: AIST, AIST - Division V, AIST - Division VI
Program Organizers: Luis Ruiz-Aparicio, Duferco Farrell Corporation, Farrell, PA 16121 USA; Dengqi Bai, IPSCO Inc., Muscatine, IA 52761 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Tuesday AM — Room: La Galerie 3
September 28, 2004 — Location: Marriott New Orleans Hotel

Session Chair: Dengqui Bai, IPSCO Steel Inc., R&D, Muscatine, IA 52761 USA

8:30 AM
Recent Advances in High-Strength, Low-Carbon, Precipitation-Strengthened Ferritic Steels: *Semyon Vaynman*[1]; *Dieter Isheim*[1]; Morris E. Fine[1]; David N. Seidman[1]; Shrikant P. Bhat[2]; [1]Northwestern University, Dept. of Matl. Sci. & Engrg., 2220 Campus Dr., Evanston, IL 60208-3108

USA; [2]Ispat Inland Inc., R&D, 3001 E. Columbus Dr., MC 0-000, E. Chicago, IN 46312 USA

Low-carbon, ferritic, precipitation-strengthened steels are being investigated seeking ever-increasing yield strengths with excellent fracture toughness properties at room temperature and 233 K. Low carbon steels containing Cu, Ni, and Al as well as NbC for grain refinement are achieving yield strengths in excess of 1000 MPa when solution treated and aged. When quenched from 1173 or 1273 K, the matrix is ferritic with no evidence for martensite. The composition of nanometer sized precipitates and their temporal evolution on aging at 773 K is investigated employing three-dimensional atom-probe (3DAP) microscopy. Stress-strain behavior versus temperature, strain rate, and aging as well as Charpy impact energy down to cryogenic temperatures are discussed. Research is supported by ONR Grant N00014-03-1-0252/P00001, Julie Christodoulou, grant officer.

8:55 AM

Precipitation in Ferrite During Isothermal Aging of X80 Steel: *Qingfeng Wei*[1]; Stephen Yue[1]; Jinbo Qu[1]; [1]IPSCO, Wong Bldg., 3610 Univ. St., Montreal, Quebec H3A 2A7 Canada

In microalloyed steels one of the strengthening mechanisms is precipitation of Nb(C, N). Steel made from scrap, however, can contain up to 0.4% Cu, which can also potentially precipitate in ferrite. Most research has shown that steel with Cu levels below 0.5% does not precipitate out Cu under normal processing conditions. In this work, the microstructure of such steels, processed by a variety of thermomechanical treatments, have been characterized by FE-SEM. At low ageing temperatures, many fine Cu precipitates were observed in ferrite compared to a few relatively large Nb containing precipitates. These results will be rationalized, and the consequences discussed.

9:20 AM

Study of Precipitation Kinetics of Copper in HSLA Steel by Small Angle Neutron Scattering (SANS): *Chandra Shekhar Pande*[1]; [1]Naval Research Laboratory, Phys. Metall. Branch, Code 6325, Washington, DC 20375 USA

Precipitation kinetic of copper in a high strength low-carbon ferrous alloy has been studied in the past mostly by field ion microscopy. These precipitates are initially coherent with the matrix and hence are difficult to detect by conventional transmission electron microscopy (TEM). We have therefore used TEM in conjunction with small angle neutron scattering (SANS) to study copper precipitation. Direct measurement from TEM micrographs and integral transform of the SANS data was used to calculate the size distribution for a variety of aging conditions. Maximum entropy principle was used to refine the distribution obtained. The role of these precipitates in hardening of the material will also be considered.

9:45 AM

Effect of Carbide Formation on the Microstructure and Texture of Warm Rolled and Annealed Low Carbon Steels with Cr and B Additions: Ilana B. Timokhina[1]; Alex I. Nosenkov[1]; John J. Jonas[2]; *Elena V. Pereloma*[1]; [1]Monash University, Sch. of Physics & Matls. Engrg., SPME, Bldg. 69, Monash Univ., Victoria 3150 Australia; [2]McGill University, Dept. of Metallurgl. Engrg., 3610 Univ. St., Montreal, Quebec H3A2B2 Canada

The development of the desirable ND fibre, which is responsible for high r-values in the warm rolled and annealed steels, has been connected to the presence in the microstructure after rolling of a high volume fraction of grains containing shear bands. These shear bands then become the preferential nucleation sites for recrystallised grains. In the current work, the effect of chromium and boron addition on the microstructure and texture formation of warm rolled and annealed extra low carbon (ELC) steel was studied. The microstructure of all the steels after warm rolling consisted of the polygonal ferrite grains with the lowest grain thickness in the ELC steel. The addition of the chromium and boron led to the formation of coarse $Cr_{23}C_6$ carbides and various fine strain-induced carbides. The latter affected the microbands thickness, dislocation density and the stored energy. As a result, the rate of work hardening and number of grains containing shear bands have increased in Cr alloyed steel leading to a higher fraction of ND fibre compared to ELC steel.

Product Application and Development: Session III

Sponsored by: AIST, AIST - Division VI
Program Organizers: E. Buddy Damm, The Timken Company, Canton, OH 44706-0930 USA; Amy Bailey, TXI - Chaparral Steel, Midlothian, TX 76065 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Tuesday AM — Room: La Galerie 5
September 28, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Roger Pradhan, International Steel Group, Bethlehem, PA USA; Brian Nelson, Dofasco Inc., Hamilton, OH L8N 3J5 Canada

8:30 AM

A Comparison of Niobium and Vanadium HSLA Steels for Light Gauge High Strength Strip: *Clare Louise Wynn*[1]; Peter Evans[2]; Russell Evans[1]; Mark Evans[1]; [1]University of Wales, Matls. Rsch. Ctr., Sch. of Engrg., Singleton Park, Swansea SA2 8PP UK; [2]Corus R,D&T, Engrg. Ctr. for Mfg. & Matls., Heol Cefn Gwrgan, Port Talbot, Swansea SA13 2EZ UK

Experimental laboratory hot rolling studies have been carried out on a range of steels with varying levels of niobium and vanadium micro-alloying additions. The strengthening effect of niobium produces grain refinement during hot rolling through retardation of recrystallisation while vanadium precipitates out below the final finishing temperature and causes precipitation strengthening after the completion of hot rolling. The lower rolling loads seen during experimental laboratory hot rolling of the vanadium chemistries give scope for extension of the existing niobium-HSLA steel product range to lighter gauges and increased widths. At higher strength levels where the strengthening efficiency of niobium begins to saturate, dual additions of niobium and vanadium may be appropriate - the relative amounts required for a particular strength level need further investigation and will be influenced by the final property requirements, ease of hot rolling and overall alloying cost.

8:55 AM

Mill Chatter: *Stephane Gouttebroze*[1]; Michel Abikaram[1]; Jean Perret[1]; [1]Vai Clecim, DTI, 51 rue Sibert, BP 154, St. Chamond 42403 France

In the cold rolling industry, Mill chatter is at the same time a well known problem (studied for many years) and an unsolved problem (no industrial solution is widely spread). This situation proves the complexity of the phenomenon. In this context, ARCELOR Mardyck, Irsid and VAI-Clecim decide to join their efforts for investigating the Mill chatter. The paper presents an experimental and numerical study of the phenomenon. The results of this study are the definition of dedicated rolling condition monitoring, a new mill design and innovative anti-chatter systems. These anti-chatter systems will be implemented on an industrial ARCELOR site in late 2004.

9:20 AM

In-Process Monitoring of Pinch Welding: An Investigation of a Bond Quality Indicator: *Daniel A. Hartman*[1]; Michael G. Smith[1]; [1]Los Alamos National Laboratory, Los Alamos, NM USA

This work investigates the feasibility of developing an in-process, non-destructive evaluation (NDE) system for pinch welding of stainless steel tubes. Acoustic emission (AE) was used as a in-process metric for monitoring pinch weld bond quality. A design of experiments was conducted in which good (primarily solid-state cond with minimal melting), hot (excessive melting and expulsion), and cold (no metallurgical bond) welds were made. Post weld metallography was performed on each weld in order to establish bond quality. In-process data (current, voltage, force, and acoustic emission) were collected for each weld. The AE data were explored through a variety of feature descriptors and, in some cases, fused with the machine data in an attempt to find a correlation with bond quality. Previous work[1-4] was inconclusive as to whether acoustic emission is a useful in-process metric for monitoring pinch weld quality. The current work demonstrates that advances in computation power, signal processing routines, and data analysis techniques provide the necessary tools to properly mine the in-process data, and that bond quality can be determined in-situ using a combination of machine process data and acoustic emission data. [1]C. W. Pretzel and A. G. Beattie, Acoustic Emission Chracaterization of Pinch Welds, SAND85-8890, Unclassified, 1986. [2]A. G. Beattie and C. W. Pretzel, J. of Acoustic Emission, 5, 172 (1986). [3]A. F. Reichman, Correlation of Pinch Weld Strength with Acoustic Emission, Proceedings of the 46th DAMSUL Committee Meeting, Oak Ridge, TN, June 5-6, 1985. [4]A. E. Clark, Feasibility Study of Acoustic Emission Monitoring of Pinch Welding Tritium Reservoir Fill Stems at the Savannah River Site, WSRC-MS-90-297, Unclassified,1990.

9:45 AM
Application of TRIP Steel for Enhanced Durability of a Shock Tower Assembly: *R. Mohan Iyengar*[1]; S. Laxman[2]; C. Roche[3]; M. Amaya[3]; [1]SeverStal N A; [2]Quality Engineering and Software Technologies; [3]Daimler-Chrysler Corporation

The application of TRIP 590 for improved durability of a shock tower assembly is examined. The proposed TRIP steel design of the assembly offers a 13% weight reduction opportunity. Detailed linear finite element analyses are conducted to evaluate the shock load-displacement response of baseline and proposed CAE models. We also examined the fatigue life of the proposed model with HSLA 350 steel in lieu of TRIP 590. The results of the analyses are used to conduct fatigue analysis using nCode with realistic time history of load based on proving ground data. The calculated fatigue lives are much better for the proposed model with TRIP 590. Results also show that the downgaging is not possible with HSLA 350. To understand the role of material nonlinearity, we conducted nonlinear CAE analysis of the models. Nonlinear analyses confirm the enhancement in durability provided by TRIP 590 over HSLA 350.

10:10 AM Break

10:30 AM
Boron Steels for Superior Durability in Automotive Structures: *R. Mohan Iyengar*[1]; J. Chen[1]; S. Laxman[2]; K. Knop[3]; S. Venkataratnam[3]; [1]SeverStal N A; [2]Quality Engineering and Software Technologies; [3]Daimler-Chrysler Corporation

Boron steels offer exciting opportunities for enhanced durability and crash performance at significant weight savings in automotive structures. In this paper, the authors will demonstrate the viability of boron steels for a variety of automotive components, including frame and chassis parts and body structure parts. In all the cases, emphasis will be placed on demonstrating the enhanced durability of the boron-steel components in relation to those made with traditional high strength steels. The significant weight savings will also be demonstrated.

10:55 AM
Effect of the Initial Texture on the Texture Evolution of IF Steel: *Gyosung Kim*[1]; Kyooyoung Lee[1]; Hyotae Chung[2]; [1]POSCO, Sheet Products & Process Rsch. Grp., 1, Goedong-dong, Pohang, Gyeongbuk 790-785 Korea; [2]Kangneung National University, Dept. of Metall. & Matls. Sci., Kangneung, Kangwon 210-702 Korea

Twice-repeated cold rolling and annealing process was applied to the Ti bearing IF steel. The 2nd cold rolling ratio should be higher than 50% for the completion of recrystallization during the following 2nd annealing process, and the mean plastic strain ratio(rm) value of 3.0 ~ 3.5 could be obtained by applying the 2nd cold rolling ratio over 70% in the Ti bearing IF steel. The comparison of texture component by ODF was made for the above material with the conventional IF steel which was produced by cold rolling and annealing using a hot band. The initial texture prior to 2nd cold rolling had the typical strong ã-fiber of annealed IF steel and was continuously strengthened by the following cold rolling and annealing process, which was also compared with the results calculated by the polycrystalline plasticity for the simulation of the texture development and rm value.

11:20 AM
Thermodynamic Modelling of Precipitation Reactions in Novel Interstitial Free (IF) Strip Steels: *Shgh Woei Ooi*[1]; G. Fourlaris[1]; [1]University of Wales, Sch. of Engrg., Singleton Park, Swansea SA2 8PP UK

Microalloying additions in IF Steels stabilise the interstitial elements present with a view of increasing ultimately the formability of the steel. However, the precipitates forming and the solute left in the matrix play a major role on recrystallisation and grain growth of the steel. In this study the volume fractions of precipitated species forming and the interstitial element(s) left in the ferrite matrix, in two novel interstitial free (IF) steel grades (a Ti only and a combined Ti-V grade) under equilibrium conditions, at various annealing temperatures are calculated by employing the MT-DATA thermodynamic modelling software. Moreover, metallographic characterisation and grain size measurements assess the effect of precipitation and solute left in the matrix. It has been identified that Ti(C,N) could form, however their composition could vary with annealing temperature. It has also been confirmed the crucial role of Ti additions in controlling the carbide precipitation within ferrite for both IF grades.

Rhenium and Rhenium Containing Alloys: Rhenium Containing Alloys

Sponsored by: TMS - Structural Materials Division, TMS - SMD-Refractory Metals Committee
Program Organizer: Todd A. Leonhardt, Rhenium Alloys, Research and Development, Elyria, OH 44036-0245 USA

Tuesday AM — Room: Grand Ballroom J
September 28, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Mehmet Uz, Lafayette College, Chem. Engrg., Easton, PA 18042 USA; Todd Leonhardt, Rhenium Alloys, R&D, Elyria, OH 44036-0245 USA

8:30 AM
Effects of Re on the Temporal Evolution of the Microstructure of a Ni-Al-Cr Alloy: Kevin E. Yoon[1]; Ronald Noebe[2]; *David N. Seidman*[1]; [1]Northwestern University, Matls. Sci. & Engrg., Cook Hall, 2220 Campus Dr., Evanston, IL 60208-3108 USA; [2]NASA, John H. Glenn Rsch. Ctr., 21000 Brookpark Rd., Cleveland, OH 44135 USA

We are studying the effects of Re on the temporal evolution of a Ni-Al-Cr-Re alloy aged at 1073 K, for times ranging from 0 to 256 hours, employing conventional transmission electron microscopy (CTEM) and three-dimensional atom-probe (3DAP) microscopy. The gamma prime precipitates (L12 structure) in the gamma matrix (FCC) have a spheroidal morphology for all aging times due to the near zero value of the misfit parameter between the matrix and precipitates. The temporal evolution of the mean precipitate radius, mean number density of precipitates, and the supersaturations of Al, Cr, and Re in both the FCC matrix and gamma prime precipitates are all followed using CTEM and 3DAP microscopies; the time laws for these three quantities are determined and compared to classical LSW theory for coarsening. The precipitate size distributions (PSDs) are also measured and compared with LSW theory. Research supported by NSF and NASA.

9:00 AM
Wear and Oxidation Resistant Rhenium Alloys: Their Applications and Properties: *Robbie J. Adams*[1]; [1]Honeywell, ESA, 1300 W. Warner Rd., M/S1207-5v, Tempe, AZ 85284 USA

Honeywell uses rhenium (Re), a refractory metal, for some of its very high temperature Aerospace applications. We have developed new wear and oxidation resistant rhenium (Re) alloys for other applications. For example use of Re as a coating can provide high wear resistance and high impact loading capability. The most important barrier to the use of Re for this application and other conventional wear applications is its poor oxidation resistance. Many potential applications include elevated temperature in an air environment. Unfortunately in air Re oxidizes as its temperature at approximately 640°F and produces a volatile oxide. At higher temperatures it may oxidize catastrophically. However the literature reviewed, as well as previous tests at Honeywell, indicate that Re in neutral or reducing environments, is highly erosion and wear resistant. These properties are evident at elevated temperatures as well as room temperature. We found our rhenium alloys approached or exceeded the wear resistance of conventional coatings such as nitriding, carburizing and tungsten carbide. In addition we were able to develop alloys with oxidation resistance approaching that of stainless steels up 1200°F. Finally preliminary testing indicates some of our formulations increase the thermal conductivity at the surface of the alloys. We will present data about applications of the alloys and their properties. We will also discuss alternative manufacturing methods of these alloys.

9:30 AM
Molybdenum-41% Rhenium Alloy Fabrication and Characterization: *E. K. Ohriner*[1]; E. P. George[1]; M. L. Santella[1]; J. R. DiStefano[1]; J. P. Moore[1]; J. F. King[1]; [1]Oak Ridge National Laboratory, Metals & Ceram. Div., PO Box 2008, Bldg. 4508, MS 6083, Oak Ridge, TN 37831 USA

An arc melted Mo-41%Re alloy has been selected for use in components in alkali metal thermal to electric conversion (AMTEC) cells. The good mechanical properties, fabricability, liquid-metal corrosion resistance, and resistance to low-pressure oxygen of molybdenum-rhenium alloys best meet the requirements for this application. The Mo-41%Re alloy was selected for its low thermal conductivity, while avoiding a composition likely to precipitate potentially undesirable phases. The alloy was fabricated by arc-melting, extrusion and hot and warm rolling. A number of components for AMTEC cells were produced for testing. Assessments of the properties of Mo-41%Re alloy were made to provide recommended data for design purposes. Mechanical properties, oxidation behavior, aging behavior and thermal properties in the temperature range up to 900°C are presented. Welding and brazing behavior of the material and resistance to liquid sodium metal are also discussed.

10:00 AM
Increased Processing Options and Properties of Molybdenum-Rhenium Alloys as a Result of Powder Modification: *Don Mitchell*[1]; Todd Leonhardt[1]; Jim Downs[1]; [1]Rhenium Alloys, Inc., 1329 Taylor St., PO Box 245, Elyria, OH 44036-0245 USA

Recent advancements in powder modification and manufacturing techniques have lead to enhanced properties of molybdenum-rhenium (Mo-Re) components. This enhancement is the result of improved processing developments for the manufacturing of composite Mo-Re powders. Generally, techniques for compaction of traditionally blended Mo-Re powders involve, pressing, pre-sintering, sintering and rolling, but the use of composite Mo-Re powders can allow for the two-step sintering method to be replaced by a lower temperature, one-step operation. This measurable decrease in temperature requirements and a decrease in the need for segregation-control provide a reduction in processing-cost while simultaneously increasing processing options. A focus on the microstructural and mechanical properties in respect to traditionally blended and composite starting powders will be discussed in great detail.

10:30 AM Break

10:40 AM
Properties of Laser Additive Manufactured (LAMSM) Rhenium-Tungsten Alloy Structures: *Frank Arcella*[1]; Todd Leonhardt[2]; Dave Abbott[1]; Khershed Cooper[3]; [1]AeroMet, 7623 Anagram Dr., Eden Prairie, MN 55344 USA; [2]Rhenium Alloys Inc., 1329 Taylor St., Elyria, OH 44035 USA; [3]Naval Research Laboratory, Matls. Sci. & Tech. Div., Washington, DC USA

The AeroMet Laser Additive Manufacturing (LAM) process has been employed to fabricate rhenium and rhenium-tungsten alloy shapes and test structures. The LAM process and the fabrication of rhenium shapes will be described. Examples will be shown where LAM could be employed to economically produce near net shape rhenium shapes in minutes without molds or dies. Alloying in process from elemental powder blends produced two rhenium-tungsten alloys. The resulting Re-W alloy shapes were cold rolled and annealed to a 30% reduction in order to enhance microstructure and performance properties. The resulting material was characterized for microstructure, alloy constituent distribution, and mechanical property performance at elevated temperatures. These results will be described in detail.

11:10 AM
Tungsten 25% Rhenium Tooling for Friction Stir Welding: *James Downs*[1]; Todd Leonhardt[1]; [1]Rhenium Alloys, Inc., 1329 Taylor St., PO Box 245, Elyria, OH 44036 USA

The material considered ideal for use in tooling in friction stir welding (FSW) applications is Tungsten 25% Rhenium, due to its enhanced physical properties. These include a high modulus of elasticity, excellent ductility, a low ductile to brittle transition temperature (DBTT) and a very high re-crystallization temperature. The material for this tooling has gone through a raped evolution since its inception, transitioning from a low-density rod possessing less than desirable properties, to high density, high strength material as used in today's FSW tools, with applications as diverse as the welding of large, thick sections of various steels to welding of titanium for a wide range of industries. A discussion of the processing, properties and microstructures of W 25%Re, pure W and Thoriated W will be presented in conjunction with a review of early production methods of W 25%Re rods, to the W Re alloys of today.

11:40 AM
To Be Announced: *Bill W. Buckman Jr.*[1]; [1]Refractory Metals Technology, PO Box 10055, Pittsburgh, PA 15236-6055 USA

Abstract not available.

Roll Technology: Maintenance and Inspection

Sponsored by: AIST, AIST - Division V
Program Organizers: Ron Webber, Dofasco Inc., Hamilton, Ontario L9G 4T1 Canada; Phil Perry, NSC/PMD Nippon Steel, Plant & Machinery Division, Crown Point, IN 46307 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Tuesday AM — Room: La Galerie 1
September 28, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Jim Valentine, United Foundries, Canton, OH 44705 USA; Thomas P. Adams, Akers National Roll, Avonmore, PA 15618-9728 USA

8:30 AM
TOPOCROM® - A Superior Method to Texture Work Rolls: *Manfred Haissig*[1]; Greg McLean[2]; [1]M.H. Consulting, 4839 Huddersfield Dr., Harrisburg, NC 28075 USA; [2]TCT Industries, Inc., 324 Breezewood Dr., Bay Village, OH 44140-1235 USA

Steel makers are constantly searching for means to reduce the conversion cost of their products and to increase the productivity of their mills to cut fixed cost. Product quality improvement is an item of that equation. Part of their research is to develop a superior product compared to that of their competitors to gain market share and higher prices. TOPOCROM textured work rolls for cold mills and skin pass mills are one means to achieve such goal. The benefits to be gained by employing TOPOCROM textured rolls are many from the standpoint of strip surface quality, the reduction in manufacturing cost to the producing steel plant and the reduction in the manufacturing cost to the manufacturer that uses the strip to produce a consumer product. This paper briefly describes and compares the existing texturing methods, explains the Topocrom process and discusses the cost benefit for steelmakers and steel users when using the Topocrom texture rather than SBR or EDT textures.

8:55 AM
Roll Repair by Submerged Arc Welding: *Dennis Hetzner*[1]; [1]The Timken Company, Advd. Matls., 1835 Dueber Ave. SW, PO Box 6930, Canton, OH 44706 USA

Timken Industrial Services LLC (TIS), Niles, Ohio, is a wholly owned subsidiary of The Timken Company. TIS provides steel mills with several repair services such as Bearing Remanufacturing, Chock and Bearing Housing Rebuilds, Mill Maintenance Programs, Reclamation Services, and Roll Repair. Typically, Roll repair consists of rebuilding the bodies of the rolls using the submerged arc welding process. While new rolls are frequently made from medium carbon alloy steel or low carbon steel, the repair process is not limited to this narrow range of materials. By using proper welding procedures, alloys such as 410 and 420 stainless steel can be clad on rolls subjected to moderate wear or moderately elevated temperature applications. In environments experiencing higher temperatures or abrasive wear, several types of hot worked die steel alloys can be used to rebuild mill rolls. One common clad used for roll repair is similar to H11 die steel. Another alloy having a high Columbium content has been found to have good resistance to elevated temperature oxidation and very good wear resistance. The quality of the welded clads as evaluated by ultrasonic testing will be compared to wrought alloy steels. Other metallurgical properties of the clads will be discussed.

9:20 AM
Roll Department Modernization: *David W. Johnson*[1]; Roy Dominguez[1]; Judson F. Martt[2]; [1]California Steel Industries, 14000 San Bernardino Ave., Fontana, CA 92335 USA; [2]J. F. Martt & Associates

In the mid 1990s, CSI had finished commissioning a new continuous pickle line. To position CSI for 2000 and beyond, the facility round out plan also included rebuilding the 5-stand cold reduction mill and constructing a second hot dip galvanizing line. To support the doubling of cold reduction capacity, consolidation and upgrade plans were formulated for the Galvanize and Cold Sheet Roll Department. This paper will outline the enhancements to grinding, roll preparation and logistics equipment. Improvements to quality and shop productivity will be highlighted.

9:45 AM Break

10:00 AM
The Application and Benefits of New Saddle Type Roll Micrometer Technology: *William E. Mellander*[1]; Susan Harford[1]; [1]Harford Industries, Inc., Epac Div., 1635 Starwood Dr., Chesterton, IN 46304 USA

Diagnosing and pinpointing mill problems with this saddle-type roll micrometer which measures roll profile, roll surface temperature, and roll diameter; improvements in roll profiling capabilities, roll shop management, and in mill safety. This has resulted in improvements in roll shop management with auditing and monitoring of machine performance, operator performance, roll performance. Sophisticated data acquisition and transfer to help users meet and document quality standards. Operator safety with Epac's patent-pending compact and light-weight design. New measurement capabilities and troubleshooting applications with unique design.

10:25 AM

Evolution of Roll Inspection Systems to Meet Changes in Roll Technologies and Roll Shop Practices: *Anthony Payling*[1]; [1]SARCLAD

Since the introduction of automated roll inspection units in the early 1980's, roll technology and roll shop practices have changed dramatically. Rolls have changed in material composition and manufacturing, roll shops have steadily reduced manning levels, and the explosion in the uses of computers has transformed information technology. To meet these new demands roll inspection has also changed and now includes both surface and sub surface inspection. The operator interface has changed with the use of graphics, and results are shared with other management systems. These developments are discussed, and roll makers and roll users will be asked to speculate on future trends in this critical area.

10:50 AM

EDT - Roll Texturing Technology as a Base for Modern Surface Structures in Automotive Cold Mill Flat Products: *Peter Vinke*[1]; Michael Utsch[1]; [1]Waldrich Siegen Werkzeugmaschinen GmbH, Daimlerstrasse 24, Burbach 57299 Germany

Purpose: The automotive industry demands a certain surface roughness on the sheet in order to have smooth deep drawing and lacquering operations. Deep drawing requires a coarse structure whereby oil pockets are formed to prevent the metal sheet from 'cold welding' to the die shoe tool. Lacquering requires a fine structure to achieve a surface finish with a high quality; and a defined roughness to have an excellent cling to the sheet. An optimum compromise between both requirements is strived for in practice. This means that a certain roughness factor with a higher uniformity over the sheet surface and a higher reproducibility must be provided. WALDRICH SIEGEN has developed an electrode erosion machine that provides the solution to these requirements. After grinding the roll texturing is performed on a separate Electronic Discharge Texturing Machine (EDT-machine) through CNC controlled spark erosion. Integrated in the EDT machine is a super finishing equipment which is integrated in machine and CNC control. This solution is used for calibrating the texture and especially the peak counts after final texturing. It is world wide the first EDT machine design for optimizing and calibration stochastic textures to reach the best roll performance under rolling conditions. EDT - Methodology: A generator switches on the erosion impulse. The conducting particles in the dielectric oil form a dipolar bridge, which produces intermittent charge of current to be passed onto the roll. A bowl shaped particle is brought to its melting point and a gaseous by product bubble is formed at the discharge duct area. After the erosion impulse is completed, the discharge duct collapses and the melted particle are expelled. A trough-shaped surface structure remains. Comparing the blasting and EDT methods with regard to the distance of peaks from one another, EDT is significantly higher. Texturing results: The texturing process results can be programmed and reproduced with great regularity and narrow tolerances. Comparing blasting and EDT methods with regard to the distance of peaks from one another, EDT is significantly higher Summary: EDT textured thin sheets distinguish through a stochastic roughness structure with a defined formation isolated from each other of hydrostatic lubrication bore relief, which are transformed onto the thin sheet during regrinding in the skin pass mill stand. In comparison to other surface textures the EDT thin sheets show excellent tribological conditions with low coefficient of friction at simultaneously high contact stand voltage without any cold welding between transforming tool and sheet surface. The good transformation results correlate with the 3D surface parameters, for which the percentage contact area of open and closed blank surfaces and rather volume can be stipulated. The varnish results show that depending on varnishing system and application there are clear connections between thin sheet texture and the top spreading structure. EDT textures help to create an excellent appearance of the varnish. Also in regard to the structure parts of longer wave lengths, which are responsible for the so-called «orange peel effect», the EDT texture can be described as advantageous. Other stochastic and deterministic texturing processes partly show similar results for tribological transformation behaviour or optical varnish results, but only the EDT process can create textures which have extremely high peak numbers (even at high average peak-to-valley heights) and therefore fulfil the demands of the automotive industry in regard to plasticity and varnish ability.

11:15 AM

Nickel Aluminide Intermetallic Alloy Rolls Energy Benefits - Summary of Large-Scale Demonstration Project and Update: *Tony Martocci*[1]; Peter Angelini[2]; Michael Santella[2]; Vinod Sikka[2]; John Mengel[3]; [1]Consultant, (Retired BSCO); [2]Oak Ridge National Laboratory, Oak Ridge, TN 37831 USA; [3]ISG Burns Harbor Plate

Nickel aluminide intermetallic alloys have been of interest for years because of their high temperature strength and wear resistance. Difficulty in the fabrication and joining of this alloy has been a major factor in preventing its commercialization. This presentation will review the details of a large-scale demonstration project involving 101 nickel aluminide rolls in the austinitizing furnace at ISG Burns Harbor Plate. Partial funding was obtained from the U.S. Department of Energy, and technology was developed by Oak Ridge National Laboratory. Discussion will include the development of welding procedures for joining nickel aluminide intermetallic alloys with H-series austenitic alloys, development of commercial cast roll manufacturing specifications, and the production of 115 rolls by two suppliers. Also included will be the performance of these rolls, other new furnace equipment installed during the demonstration project, and the energy reduction with these rolls as part of an overall energy-efficient fur nace system. An update of roll/furnace performance one year after project completion will be provided.

The Accelerated Implementation of Materials & Processes: The Design-Materials Interface: Closing the Loop

Sponsored by: TMS - Structural Materials Division, TMS - ASM/MSCTS-Thermodynamics & Phase Equilibria Committee, TMS - EMPMD/SMD-Chemistry & Physics of Materials Committee, TMS - MPMD-Computational Materials Science & Engineering-(Jt. ASM-MSCTS)

Program Organizers: Rollie E. Dutton, Air Force Research Laboratory, AFRL/MLLMP, WPAFB, OH 45433 USA; John E. Allison, Ford Motor Company, Materials Science and Advanced Engineering, Dearborn, MI 48124-2053 USA; John J. Schirra, Pratt & Whitney, East Hartford, CT 06108 USA; Axel van de Walle, Northwestern University, Materials Science and Engineering, Evanston, IL 60208-3108 USA

Tuesday AM Room: Mardi Gras Ballroom H
September 28, 2004 Location: Marriott New Orleans Hotel

Session Chair: John J. Schirra, Pratt & Whitney, E. Hartford, CT 06108 USA

8:30 AM

Accelerated Insertion of Materials - Heat Treatment of Forged Superalloy Disks: *Daniel G. Backman*[1]; Deb D. Whitis[2]; Michael F. Henry[3]; Dan Wei[1]; Youdong Zhou[3]; Dominic Gao[3]; Peter M. Finnigan[3]; [1]GE Aircraft Engines, MD 36807, 1000 Western Ave., Lynn, MA 01910 USA; [2]GE Aircraft Engines, One Nuemann Way, Cincinnati, OH 45215 USA; [3]GE Global Research Center, One Rsch. Cir., Niskayuna, NY 12309 USA

Material and process development for aircraft engines is a long and costly undertaking that often extends upward to fifteen years. DARPA's Accelerated Insertion of Materials (AIM) initiative was formulated to reduce this cycle time by up to 50% through the application of materials modeling and systems engineering tools. At GE, the program has included research to establish linked models that simulate materials processes and predict materials microstructures and properties. By combining such models with methods for determining uncertainty, the AIM approach can account for variations in processing history, microstructural features, and both measurement and modeling errors. AIM is developing a new methodology for predicting material behavior early in the development process with reduced reliance on mechanical tests and tighter linkage to concurrent design engineering analyses. This presentation will provide an overview of the AIM system, highlights of accomplishments of GE's effort under the DARPA AIM program, and the status of AIM within GE Aircraft Engines. These findings will include a description of its application to analyze the effects of heat treatment on the mechanical properties of a forged nickel-based superalloy.

8:50 AM

The Accelerated Development of High Fatigue Performance Cast Aluminum Alloys for Automotive Applications: *A. Shyam*[1]; X. Zhu[1]; Y. N. Picard[1]; J. W. Jones[1]; J. E. Allison[2]; S. M. Yalisove[1]; [1]University of Michigan, Matls. Sci. & Engrg., 3062 H H Dow, Ann Arbor, MI 48109 USA; [2]Ford Motor Company, Scientific Rsch. Labs., Dearborn, MI 48121 USA

The useful fatigue life of cast aluminum alloys is dependent on the growth rates of small cracks that most commonly initiate from pre-existing porosity. The influence of parameters such as temperature, load-ratio, alloying, heat-treatment and microstructure on the growth rate of these cracks is not well understood. Additionally, determination of the growth rates of these cracks is problematic, especially at elevated temperatures. These factors hinder the accelerated development of automotive alloys with improved fatigue performance. The small crack growth behavior of several cast aluminum alloys was investigated. Cracks were initiated from micronotches made by femtosecond pulsed lasers and tracked optically. A mechanistic crack growth law has been developed to predict small crack growth in cast aluminum alloys as a function of parameters such as temperature and maximum stress by utilizing the known tensile properties. The crack growth rate has been found to be related to the plasticity at its tip. Implications of these results for the accelerated development of high fatigue performance cast aluminum alloys will be discussed.

9:10 AM
Parametric Formulas for Superplastically Formed Channels: *M. David Hanna*[1]; Frank G. Lee[2]; [1]GM R&D Center, Matls. & Processes, 30500 Mound Rd., M/C 480-106-212, Warren, MI 48090 USA; [2]General Motors, Dimensional Mgmt., MC 480-210-715, 30001 Van Dyke Ave., Warren, MI 48089 USA

A parametric study was conducted to determine how the design features of channel tools and forming parameters affect part thinning and forming time in the SPF (Superplastic Forming process). The Taguchi design-of-experiment method was applied to select parameter combinations, and the MARC finite element code was used to conduct sectional analysis for various combinations. The aspect ratio and entry radius had the greatest influence on blank thinning. The forming time was mostly influenced by strain rate, aspect ratio, and bottom radius. Use of DEXPERT (General Motors internally developed analytical and statistical tool) yielded formulas describing the percentage of thinning and the forming time as explicit functions of eight design and forming parameters. The formulas provide good approximations of results obtained by finite element analyses and physical experiments. Finally, design domains were established to avoid excessive part thinning.

9:30 AM
Probabilistic Modeling and Data Fusion: *D. Gary Harlow*[1]; Gregory B. Olson[2]; John J. Schirra[3]; [1]Lehigh University, Mechl. Engrg. & Mech., 19 Memorial Dr. W., Bethlehem, PA 18015 USA; [2]Northwestern University, Matls. Sci. & Engrg., 2225 N. Campus Dr., Evanston, IL 60208 USA; [3]Pratt & Whitney, Matls. & Processes Engrg., 400 Main St., M/S 114-40, E. Hartford, CT 06108 USA

Uncertainty is an integral component of modeling, experimentation, and manufacturing, and it must be adequately characterized for design and life cycle estimation and prediction. For new materials or changes in design, the available data and information are limited intensifying concerns about the magnitude and extent of the uncertainty. A methodology is presented where uncertainty, assumed to be cumulative, can be adequately managed. The proposed methodology focuses on the fusion of limited experimental data with science based modeling. The fusion is achieved through a combination of Bayesian analyses, modeling, and experimental data to improve estimations and predictions. The methodology is applied to the yield strength of a typical turbine disk alloy. The most important conclusions of the analysis are that science based modeling with data analysis greatly improves estimation and the approach allows for a significant reduction in the number of data required.

9:50 AM
Thorough Process Modelling of Cast Aluminum Alloy Components for Fatigue Life Prediction: Peifeng Li[1]; Daan M. Maijer[2]; *Peter D. Lee*[1]; Trevor C. Lindley[1]; [1]Imperial College London, Dept. of Matls., Prince Consort Rd., London SW7 2BP UK; [2]University of British Columbia, Dept. of Metals & Matls., Vancouver V6T 1Z4 Canada

The use of cast aluminium alloy components offers potential weight savings over cast iron in the automotive industry and economic advantages over wrought products in aerospace applications. However, the fatigue performance of cast aluminium components is an important consideration during casting design. The current work employs a through process modelling technique to predict the fatigue performance of a cast aluminium alloy component as a function of both its service conditions and the nuances of its multi-stage production. This was achieved by linking multiscale mathematical models that explicitly track the microstructure and stress states through the different manufacturing stages involved, including casting, heat treatment and subsequent machining operations. The final in-service performance is then simulated using sub-models which relate the tracked microstructural features and in-service stress state to fatigue life. The performance of a cast aluminium alloy automotive component was predicted using this modelling technique and compared with full-scale fatigue test results to validate the suitability of the through process modelling as a design tool.

10:10 AM Break

10:25 AM
Ti-6-4 Investment Castings for the F/A 22 - Lessons Learned: *Larry Perkins*[1]; [1]Air Force Research Laboratory/MLL, Metals, Ceram. & NDE Div., 2230 Tenth St., Ste. 1, Wright-Patterson AFB, OH 45433-7817 USA

This talk will review the use of castings for fracture critical application on the F/A 22 aircraft, the proposed benefits and technical challenges. Critical technical and non-technical issues that were not adequately addressed during selection and design will be covered. OEM, Government and vendor communication, process control capability to meet stringent fracture critical applications will be addressed. The lessons learned from this experience as well as options for improved process/materials introduction will be presented.

10:45 AM
Microstructural Characterization and Representation Using 3D Orientation Data Collected by an Automated FIB-EBSD System: Michael Groeber[2]; B. Haley[3]; M. Uchic[1]; *Dennis M. Dimiduk*[1]; S. Ghosh[4]; [1]Air Force Research Laboratory, Matls. & Mfg. Direct., AFRL/MLLM Bldg. 655, 2230 Tenth St., Wright-Patterson AFB, OH 45433-7817 USA; [2]Ohio State University, Dept. of Matls. Sci. & Engrg., Columbus, OH 43210 USA; [3]Ohio State University, Dept. of Computer Sci. & Engrg., Columbus, OH 43210 USA; [4]Ohio State University, Dept. of Mechl. Engrg., Columbus, OH 43210 USA

A new technique utilizing automated serial sectioning combined with Focused Ion Beam (FIB) and Electron Back-Scatter Diffraction (EBSD) imaging systems was implemented for collection of 3D microstructural data. Orientation data that can be used for high-fidelity modeling of grain and sub-grain structures may be obtained using the method. The technique is currently capable of sectioning a sample with inter-slice thicknesses as low as 100 nanometers and while capturing orientation maps for each slice. Automation of this technique allows for unsupervised data collection and the ability to update settings in real time. The orientation data obtained by the EBSD scans consists of each grid point's position, three Euler angles and phase-type. Reconstruction of the 3D orientation data involves combining or "stacking" the 2D slices obtained by the FIB-EBSD process. A program developed in this work, "Micro-Mesher," uses the reconstructed orientation information to define microstructural features such as grains and second phase particles. Micro-Mesher constructs grain boundaries using line and plane segments and an error-per-unit-length approach to approximate the complex grain boundaries. Important microstructural statistics are also calculated that may be used to define and characterize the 3D microstructure. Such important parameters include: grain size, number of neighboring grains, orientations and misorientations, second-phase particles size and inter-particle spacing. The 3D statistical information gained from this process has significant potential for developing high-fidelity structure representations for the multiscale material-performance prediction challenge.

11:05 AM
Accelerated Insertion of Materials - Application to Turbine Disk Creep: *David P. Mourer*[1]; Greg Bechtel[2]; Daniel G. Backman[1]; Dan Wei[1]; John J. Schirra[3]; R. Grelotti[3]; D. Harmon[3]; [1]GE Aircraft Engines, 1000 Western Ave., Lynn, MA 01910 USA; [2]GE Aircraft Engines, One Neumann Way, Cincinnati, OH 45215 USA; [3]Pratt & Whitney United Technologies, E. Hartford, CT USA

Material insertion in demanding turbine applications requires a thorough understanding and quantification of mechanical behavior that are needed for component design analyses. It is often difficult to provide such information early in the material development cycle due to the cycle time for processing material and conducting a large number of mechanical property tests. Methods developed during DARPA's Accelerated Insertion of Materials (AIM) initiative address these needs by combining data with modeling analysis to assess material and component performance. This presentation describes interim results from an Air Force funded program to determine the creep capability of an advanced nickel base superalloy and predict the creep deformation of a turbine disk. Models used in this work address heat treatment thermal response, microstructural evolution, and development of creep properties. These models, originally developed during the DARPA AIM program have been adapted for a new geometry and alloy. This presentation will provide an overview of the overall AIM methodology, and highlights of the inverse analysis in heat treatment process, the material model development and calibration, and a description of spin test validation testing.

11:25 AM
Technical Cost Modeling Accelerates Process Selection: *Krishnaswamy Sampath*[1]; [1]Consultant, 615 Demuth St., Johnstown, PA 15904 USA

Both single-melt PAM and EBM followed by a VAR step have emerged as low-cost alternatives for producing single-melt titanium alloy slabs for critical, non-aerospace applications. Technical cost modeling was used to estimate unit cost, identify principal cost drivers and perform sensitivity analyses to accelerate process selection for producing 1-inch thick Ti-6Al-4V plates for ballistic-shock resistant applications. The results showed that the principal cost drivers are raw material processing, melt processing and plate rolling. Sensitivity analyses showed that percent revert and process yield could significantly influence (or adversely impact) the estimated unit cost. A comparison of the estimated unit cost for a worst case with a best case for either PAM or EBM processed 1-inch thick plate showed a potential cost savings of 57% or 58%, respectively. The above results showed the utility of technical cost modeling approach in accelerating process selection and cost-control.

11:45 AM

The Cold Spray Processing of Metals: *Prateek Sachdev*[1]; F. H.(Sam) Froes[1]; Sunil Patankar[1]; Rick Blose[2]; Anatolii N. Papyrin[2]; [1]University of Idaho, Matls. Sci. Engrg. Dept., Inst. for Matls. & Advd. Processes, Office of Director, McClure Bldg., Rm. 437, Moscow, ID 83843 USA; [2]Ktech Corporation, 2201 Buena Vista SE, Ste. 400, Albuquerque, NM 87106-4265 USA

Cold spraying (CS) is a material depositions process in which a coating is formed by exposing a substrate to a high velocity jet of solid-phase particles. The process appears to have excellent potential for the production of monolithic near net shapes, coated concepts and as a repair technique; particularly for reactive metals. For many applications monolithic metals produced by cast and wrought (ingot metallurgy, I/M), cast, powder metallurgy (P/M) or other conventional techniques adequately meet design requirements in industries as diverse as aerospace, automotive, sporting goods etc. However advanced concepts include tailoring of the various regions of a component to meet the design requirements in that specific location - for example integral disc-blade gas turbine engine components can feature chemistry/microstructure in the bore which optimize low cycle fatigue behavior while creep performance is enhanced in the blades. The cold spraying process have been successfully used for many materials at much lower temperatures as compared to the conventional thermal spray processes.

Titanium for Healthcare, Biomedical, and Dental Applications: Fatigue and Wear

Sponsored by: TMS - Structural Materials Division, Japan Institute of Metals, TMS - SMD-Titanium Committee, TMS - SMD-Corrosion and Environmental Effects Committee-(Jt. ASM-MSCTS)

Program Organizers: Carl Boehlert, Alfred University, School of Ceramic Engineering and Materials Science, Alfred, NY 14802 USA; Dhanesh Chandra, University of Nevada, Metallurgical and Materials Engineering, Reno, NV 89557 USA; Masahiko Ikeda, Kansai University, Department of Materials Science and Engineering, Suita, Osaka 564-8680 Japan; Mitsuo Niinomi, Toyohashi University of Technology, Department of Production Systems Engineering, Toyohashi 441-8580 Japan

Tuesday AM — Room: Mardi Gras Ballroom D
September 28, 2004 — Location: Marriott New Orleans Hotel

Session Chair: Carl Boehlert, Alfred University, Sch. of Ceram. Engrg. & Matls. Sci., Alfred, NY 14802 USA

8:30 AM Invited

Cyclic Deformation Behaviour and Fatigue Induced Surface Damage of Titanium Alloys in Simulated Physiological Media: *Christian Leinenbach*[1]; Berthold Schwilling[1]; Dietmar Eifler[1]; [1]University of Kaiserslautern, Inst. of Matls. Sci. & Engrg., Gottlieb-Daimler-Strasse, D-67663 Kaiserslautern Germany

Titanium and its alloys are well known materials used for medical applications because of their high mechanical strength, low specific weight, good corrosion resistance and biocompatibility. As implant materials they have to sustain a combination of complex mechanical and biological loading in the human body. In the present investigation, the cyclic deformation behaviour and fatigue induced surface damages of commercially available titanium alloys (cp-Ti, Ti6Al4V, Ti6Al7Nb) is characterized in axial stress controlled load increase and constant amplitude tests as well as in rotating bending tests. All tests were performed in Ringer's solution. In axial tests, in addition to single step loading at R=-1 load patterns as they occur during standard human walking were used to generate more realistic loading conditions. The cyclic deformation behaviour was characterized by mechanical hysteresis measurements. Fatigue induced surface damages were detected using electrochemical techniques and correlated with microstructural investigations.

8:55 AM

Improvement in Fatigue Characteristics of Newly Developed Beta Type Titanium Alloy for Biomedical Applications by Thermo-Mechanical Treatments: *Toshikazu Akahori*[1]; Mitsuo Niinomi[1]; Hisao Fukui[2]; [1]Toyohashi University of Technology, Dept. of Production Sys. Engrg., 1-1, Hibarigaoka, Tempak-cho, Toyohashi, Aichi 441-8580 Japan; [2]Aichi-Gakuin University, Dept. of Dental Matls. Sci. Sch. of Dentistry, 1-100, Kusumoto-cho, Chikusa-ku, Nagoya, Aichi 464-8650 Japan

Implant instrumentations like bone plates, screws and nails, artificial spines, and artificial femoral and hip joints are used under fatigue conditions and sometimes failed due to monotonic loading, fatigue and corrosion fatigue. Mechanical performance, in particular, tensile, and plain and fretting fatigue performances are very important factors for titanium alloys for biomedical applications. A new beta type titanium alloy composed of non-toxic and non-allergic elements like Nb, Ta, and Zr, Ti-29Nb-13Ta-4.6Zr, has been recently developed in order to achieve lower Young's modulus and excellent mechanical performance. Fatigue performances of an alloy are important mechanical properties to confirm the reliability as metallic biomaterials. It is well-known that these properties are changed for titanium alloys according to the microstructures obtained by heat treatments or thermo-mechanical treatments. Therefore, tensile and fatigue properties of newly developed beta-ntype titanium alloy, Ti-29Nb-13Ta-4.6Zr, conducted with various thermo-mechanical treatments were investigated in this study.

9:20 AM

Evaluation of Orthorhombic+Body Centered Cubic Ti-Al-Nb Alloys for Biomedical Applications: *Christopher John Cowen*[1]; R. Jaeger[2]; M. Niinomi[3]; T. Akahori[3]; C. J. Boehlert[1]; [1]Alfred University, Ceram. Engrg. & Matls. Sci., Grad. Student Mailbox, McMahon Bldg. Rm. 352, Alfred, NY 14802 USA; [2]Biologische und biomedizinische Materialien und Implantate, Fraunhofer Institut für Werkstoffmechanik IWM, Freiburg 79108 Germany; [3]Toyohashi University of Technology, Dept. of Production Sys. Engrg., Toyahashi 441-8580 Japan

To date the material of choice used in implants is titanium-vanadium-aluminum (Ti-V-Al) alloys because of their excellent biocompatibility and their combination of high specific strength, corrosion resistance, low density, good ductility and elastic modulus, oxidation resistance, conventional processability, fatigue strength, and fracture toughness. However, V is a potentially toxic element; therefore, other alloying elements are currently being examined. In particular substitution of niobium (Nb) for V is attractive as this does not result in degradation of several mechanical properties. In this work the physical metallurgy of Ti-Al-Nb alloys, in particular Ti-17Al-33Nb(at.%) and Ti-22Al-28Nb(at.%) will be compared to those for Ti-Al-V alloys. The mechanical properties of interest are RT strength and fatigue resistance as well as elastic modulus. S-N curves will be presented for tests performed at RT in air as well as in Ringer's solution for stresses between 35%-75% of the ultimate tensile strength. This work was supported by the New York State Office of Science and Technology for Academic Research (NYSTAR #C020080) and the National Science Foundation (DMR/INT 0134789).

9:45 AM

Mechanical Properties of Ti-4.5Al-3V-2Mo-2Fe and Possibility for Healthcare Applications: *Guna Warman*[1]; Mitsuo Niinomi[1]; Toshikazu Akahori[1]; Junichi Takeda[1]; [1]Toyohashi University of Technology, Dept. of Production Sys. Engrg., 1-1 Hibarigaoka, Tempaku-cho, Toyohashi, Aichi-ken 441-8580 Japan

This study is to review the mechanical properties of Ti-4.5Al-3V-2Mo-2Fe, a relatively low cost titanium alloy originally designed for aerospace applications, conducted with single and duplex annealing treatments in alpha+beta field, and to investigate the prospective of this alloy to be use for healthcare applications such as for wheelchairs, artificial limbs and artificial legs. It was found that single-annealed Ti-4.5Al-3V-2Mo-2Fe alloy have very high fatigue ratio (0.70-0.85) and high specific strength (210-260 MPa/g.cm-3) with a modest fracture toughness (JIC=25-35 kN/m). From the point of view of mechanical properties, it can be said that this alloy has high potential for healthcare applications among available commercial metallic materials.

10:10 AM Break

10:20 AM Invited

Subsurface Deformation and Microcrack Formation in Ti-35Nb-8Zr-5Ta-O(x) During Reciprocating Sliding Wear: Marc Long[2]; *H. J. Rack*[1]; [1]Clemson University, Sch. of Matls. Sci. & Engrg., Clemson, SC 29634-0971 USA; [2]Smith & Nephews Richards, Memphis, TN 38116 USA

Subsurface deformation and microcrack formation in Ti-35Nb-8Zr-5Ta-O(x) during reciprocating-sliding wear(RSW) has been examined. Three deformation zones, a plastic zone, a plastic shear zone and a tribolayer, progressing towards the wear surface were identified, their depth increasing with increasing apparent contact stress. Transmission electron microscopy has shown that {110} and {112} planar slip occurs throughout the subsurface deformation zone, the planar slip band spacing decreasing with increasing subsurface strain. {110}/{110}and {110}/{112} slip band intersections together with localized shear displacement and microcrack formation were also observed. Once formed the microcracks propagate along {110} slip bands, the latter reorienting as the wear surface is approached. Ultimately a featureless tribo surface layer containing cracks lying parallel to the sliding direction was observed. Finally delamination along slip bands leads to debris formation, refinement of this debris occurring during further RSW.

10:45 AM
The Effects of Accelerated Wear Testing on the Corrosion Behavior of a Ni-Ti Implantable Heart Valve Frame: Melissa Denton[1]; James C. Earthman[2]; [1]Edwards Lifesciences, One Edwards Way, Irvine, CA 92614 USA; [2]University of California, Matls. Sci. & Engrg., Irvine, CA 92697 USA

Measurement of current-potential relations under carefully controlled conditions can yield information on corrosion rates, the passivation abilities, pitting tendencies and other important information. Cyclic potentiodynamic curves were obtained to evaluate the corrosion resistance of several Nitinol samples after undergoing accelerated wear testing to 200 million cycles. The effects of the microstructure and wear testing on corrosion will be discussed.

11:10 AM
Wear Mechanism of Ti-Nb-Ta-Zr Alloys for Biomedical Applications: Shu Jun Li[1]; *Rui Yang*[1]; Shu Li[1]; Yu Lin Hao[1]; Mitsuo Niinomi[2]; Zheng Xiao Guo[3]; [1]Chinese Academy of Sciences, Inst. of Metal Rsch., Shenyang Natl. Lab. of Matls., 72 Wenhua Rd., Shenyang, Liaoning Province 110016 China; [2]Toyohashi University of Technology, Dept. of Productions Sys. Engrg., 1-1 Hibarigaoka, Tempaku-cho, Toyohashi 441-8580 Japan; [3]Queen Mary, University of London, Dept. of Matls., Mile End Rd., London E1 4NS UK

The wear behavior of β type Ti-(29, 39)Nb-13Ta-4.6Zr alloys with and without heat treatment or surface modification was investigated with pig bone, ultra-high molecular weight polyethylene (UHMWPE) and stainless steel as counterface materials using a reciprocal pin-on-disk wear device in a 0.9% NaCl solution. Wear loss was found small for tests against pig bone and UHMWPE, but was significant for test against stainless steel. The high Nb alloy shows improved wear resistance than the low Nb alloy, and the wear resistance was notably improved after oxidation treatment. Heat treatments that increase the ultimate strength and hardness of the alloys are not effective in improving wear resistance. These results were rationalized by considering the formation of a layer of Nb_2O_5, a known hard and lubricating oxide, on the surface of the alloys.

11:35 AM
Modern Medically Applied Bio-Compatible Alloys on the Titanium and Cobalt-Chromium Basis: Innola Maksyuta[1]; Valentina Lachneva[2]; [1]Physico-Technological Institute of Metals and Alloys NASU, 34/1 Vernadsky Ave., Kiev 03689 Ukraine; [2]Institute of Material Acknowledgment Problems NASU, Kiev Ukraine

Two bio-compatible alloys on the cobalt-chromium and titanium basis, new in their nature, have been elaborated recently in Ukraine. These alloys successfully passed a range of tests according to the demands of International Standardization Organization. There were such tests as: medical, biological, toxicological, technical and clinical. Both materials, that by the way are included in the register of medical products approved by the Ministry of Health of Ukraine in accordance with the level of technical characteristics can be used for casting and dismantled dentures production. Tests conducted in the Institute of Material Acknowledgment Problems of NASU proved, that the «Ceradent's» (Co-Cr Alloy) endurance is similar to oxide aluminium ceramics (Al2O3) and it exceeds the endurance of titanium alloys VT5-1, VT6, VT14, VT16. Owing to these properties, new alloy can substitute endoprosthesises that are made from these materials. Comparative tests on endurance during friction of such couples as polyethylene «Hyrulen»-titanium, polyethylene-ceramics Al2O3 and polyethylene-«Ceradent» has been conducted under conditions close to the natural. Initial roughness (asperity) of the titanium and Co-Cr-alloy was estimated at Ra=0,05mm. Constant load created by contact efforts of 5N/mm2. Slip velocity was 0,1m/s, test lasted 20 hours, environment of materials disposal was a physical solution, t- 370C. Wear out was controlled by the quantity taken during a polyethylene friction. Weight and linear variations of ceramics Al2O3, polyethylene «Hyrulen», titanium and Co-Cr alloys were also measured. The biggest wear out of polyethylene «Hyrulen» was fixed in couple with Titanium VT5-1, while wear out was followed by the friction path's appearance on the titanium circle & considerable enhancement of the surfaces roughness (asperity). In conclusion of every test cycle wear out of the titanium circle measured within 5-8 mm. Wear out of the ceramics & Co-Cr casting circles was not fixed.

3-Dimensional Materials Science: 3D Atom Probe/ Computational Methods I

Sponsored by: TMS - Structural Materials Division
Program Organizers: Marc J. De Graef, Carnegie Mellon University, Department Material Science & Engineering, Pittsburgh, PA 15213-3890 USA; Jeff P. Simmons, Air Force Research Laboratory, Materials & Manufacturing Directorate, Dayton, OH 45433 USA; George Spanos, Naval Research Laboratory, Physical Metallurgy Branch, Washington, DC 20375-5000 USA; Jonathan E. Spowart, UES Inc., Dayton, OH 45432 USA

Tuesday PM — Room: Mardi Gras Ballroom F/G
September 28, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Benji Maruyama, Air Force Research Laboratory, Matls. & Mfg. Direct., WPAFB, OH 45433-7817 USA; Michael K. Miller, Oak Ridge National Laboratory, Metals & Ceram. Div., Oak Ridge, TN 37831-6136 USA

2:00 PM Invited
Atom Probe Tomography and the Local Electrode Atom Probe: *Michael K. Miller*[1]; Sudarsanam S. Babu[1]; [1]Oak Ridge National Laboratory, Metals & Ceram. Div., PO Box 2008, Bldg. 4500S, MS 6136, Oak Ridge, TN 37831-6136 USA

The commercial introduction of the local electrode atom probe (LEAP®) has dramatically improved the ability to characterize the three-dimensional atomic-scale structure of materials. The local electrode variant of three-dimensional atom probe features a significantly larger field of view and substantially faster data acquisition rate. This atom probe tomography technique measures the spatial coordinates and the elemental and isotopic identities of the atoms in a small volume of analysis that typically contain several million atoms. The performance of this instrument will be presented with examples of solute segregation to dislocations and grain boundaries, solute partitioning to coexisting phases and phase separation in nickel base superalloys. Research at the Oak Ridge National Laboratory SHaRE User Center was sponsored by the Division of Materials Sciences and Engineering, U.S. Department of Energy, under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

2:30 PM Invited
Three-Dimensional Atom-Probe Microscopy Studies of Temporally Evolving Microstructures: *David N. Seidman*[1]; [1]Northwestern University, Matls. Sci. & Engrg., Cook Hall, 2220 Campus Dr., Evanston, IL 60208-3108 USA

Three-dimensional atom-probe (3DAP) microscopy is being applied to a wide range of systems to study the temporal evolution of the microstructure with atom-scale resolution on length scales from the subnanometer to the mesoscale. Emphasis is placed on understanding nucleation, growth, coarsening and heterophase interfacial segregation for the following systems: (1) Ni-Al-Cr alloys with Re, W, and/or Ru additions; (2) Al-Sc-Mg, Al-Sc-Zr, Al-Sc-Ti alloys; (3) TiAl with carbides, borides, and nitrides; and (4) high-strength low-alloy (HSLA) steels (1000 plus MPa) with copper and niobium carbide precipitates. In concert with the 3DAP microscopy studies we are studying the high temperature creep properties of selected Ni-Al-Cr alloys, Al-Sc-Mg, Al-Sc-Zr and Al-Sc-Ti alloys, and the yield stress and plasticity of HSLA steels at room temperature and fracture toughness at 233 K, which enables us to make structure-property correlations. Research supported by the NSF, DOE, ONR and NASA.

3:00 PM
Three Dimensional Microstructural Simulation and Micro-Stress Analysis of Polycrystalline Metallic Materials: *Yaowu Zhao*[1]; Robert G. Tryon[1]; [1]VEXTEC, 750 Old Hickory Blvd., Bldg. #2, Ste. 270, Brentwood, TN 37027 USA

Titanium and nickel-based polycrystalline materials are modeled using a statistical volume element (SVE) of three-dimensional space filling grains with each grain having unique properties. A Voronoi tessellation software program is developed to determine the geometry of the grains in the polycrystal. The software is combined with the MSC PATRAN finite element method (FEM) geometry generation software to automatically generate the SVE model. In the SVE model, each grain is assumed to have anisotropic mechanical properties with different orientations. Other unique properties at the grain level can be defined such as grain size and shape. The SVE model is automatically converted into a NASTRAN FEM with each grain being defined with multiple elements. The FEM model is executed to determine the stress distribution throughout the polycrystal. The local stress was strongly correlated with the orientation and weakly correlated with grain size and shape. The underlying mechanics for these observations is elucidated.

3:20 PM Break

3:50 PM
3D Modeling of Graphitic Carbon Foams: *Benji Maruyama*[1]; Daylond Hooper[2]; Khairul Alam[3]; Jonathan Spowart[4]; [1]Air Force Research Laboratory, Matls. & Mfg. Direct., AFRL/MLBCO, 2941 Hobson Way, WPAFB, OH 45433 USA; [2]Wright State University, Dept. of Biomed. & Indust. Engrg., OH USA; [3]Ohio University, Athens, OH USA; [4]UES Inc., 4401 Dayton-Xenia Rd., Dayton, OH 45432 USA

Abstract not available.

4:10 PM
Computational Simulation of 3D Molecular Dynamics of Novel Diamonds-Containing Nanocomposites: *Maksim V. Kireitseu*[1]; [1]Institute of Mechanics and Machine Reliability, Lesnoe 19 - 62, Minsk 223052 Belarus

The principal goal of the paper was to demonstrate an application of modern software engineering tools for modelling virtual reality and molecular dynamics of novel nanocomposites. The main technical components of presented system are 1) software and nanoengineering tools for modelling of virtual reality, molecular dynamic and 3D video images of novel diamonds-containing nanocomposites and 2) Problem tracking system to be used during modelling of virtual reality. A computational scheme and software, which utilizes neural networks and/or Microsoft.Net technique, was developed to predict properties of nano-structured materials and optimization and control of nano-devices. Developed software and IT nanoengineering tools can be used by both industrial and private single users. For commercial companies proposed technology provide better cost-effective alternative to the existing solutions for nanoengineering and modeling their virtual reality such as very expensive Silicon Graphics stations. For private users (students, professors, engineers) proposed technology and IT tools can provide simple and cost-effective solution for nanoengineering while studying, exploring virtual reality and modeling novel nanostructures and its properties leading to an innovation or a discovery. Because of using novel software and methodologies users can easily operate proposed technologies by available computers and operating systems. Also users can upgrade it by their own self-written models, if necessary.

Advancements in Mechanical Property Characterization at the Micro- and Nano-Scale: Development and Application of Mechanical Property Characterization Methods II

Sponsored by: TMS - Structural Materials Division
Program Organizers: Mike Uchic, Air Force Research Laboratory, Dayton, OH 45433-7817 USA; Kevin J. Hemker, Johns Hopkins University, Department of Mechanical Engineering, Baltimore, MD 21218 USA; Marc Zupan, University of Maryland, Baltimore, MD 21250 USA

Tuesday PM — Room: Mardi Gras Ballroom B
September 28, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: William N. Sharpe, Johns Hopkins University, Dept. of Mechl. Engrg., Baltimore, MD 21218-2681 USA; Dennis M. Dimiduk, Air Force Research Laboratory, Matls. & Mfg. Direct., Wright Patterson AFB, OH 45433-7817 USA

2:00 PM Invited
Direct Nanoscale Measurements of Material Deformation and Fracture Properties with Application to Thin Films and MEMS: *Ioannis Chasiotis*[1]; [1]University of Virginia, Mechl. & Aeros. Engrg., Charlottesville, VA 22904 USA

Microscale structures and nanophase materials require the investigation of their mechanical behavior at scales comparable or significantly smaller than the specimen size or the length-scale introduced by the material microstructure. We have developed an experimental methodology to obtain unequivocally the local deformation fields in any material system with true nanometer spatial resolution in displacements and strains using specimens of any geometry. This methodology is based on decoupled measurements of local deformations and stresses via microtension tests conducted in situ with the aid of a Scanning Probe Microscope (SPM). High-resolution surface topographies are converted into displacement and strain fields through a Digital Image Correlation (DIC) algorithm that is capable of resolving sub-pixel displacements and their first and second order gradients. Recent advances in SPM technology provided us with 1 nm true spatial (hardware) resolution using AFM tips with 1 nm radius of curvature and 12-bit AFM scan resolution. The image correlation algorithms applied here further improve the displacement resolution to a few Angstrom. Among the advantages of this methodology is that direct records of the local nanometer-level displacements and strains are obtained without the need for assumptions and models for the experimental procedure or the materials tested. Extensive experiments conducted on freestanding thin polycrystalline silicon, diamond-like carbon, and gold films will be used to illustrate the application of our AFM/DIC methodology. Young's modulus and Poisson's ratio were measured for the first time from 5x10 micron, or smaller, material domains while the local non-uniform deformation fields were also recorded in the vicinity of micron-size acute notches allowing us to resolve tensile notch stresses as high as 11.5 GPa. This presentation will also address the deterministic and stochastic aspects of failure in MEMS-scale structures and thin films. The first fracture toughness tests conducted via microtension specimens with mathematically sharp cracks will be presented along with measurements of the local deformation fields in the vicinity of cracks. Furthermore, a review of detailed studies conducted by our group to characterize the effects of stress concentration factors and local radius of curvature on failure of microscopic specimens will be discussed. The aforementioned SPM-based methodologies permit the direct study of phenomena associated with the evolution of material failure while supporting a better understanding of the issue of fatigue-failure of microdevices. Examples will highlight our ability to concurrently record local phase transformations and damage initiation during in situ AFM fatigue testing, a critical capability in elucidating fatigue mechanisms in brittle thin films.

2:30 PM
How to Accurately Measure Nanoscale Materials Properties by Tensile Testing? Effect of Offset Angle on Nanoscale Tensile Measurements: *Xiaodong Li*[1]; Xinnan Wang[1]; Wei-Che Chang[1]; Yuh J. Chao[1]; Ming Chang[2]; [1]University of South Carolina, Dept. of Mechl. Engrg., 300 Main St., Columbia, SC 29208 USA; [2]Chung Yuan Christian University, Dept. of Mechl. Engrg., 22 Pu-Jen, Pu-Chung Li, Chung-Li (32023), Taiwan China

The extremely small dimensions of nanostructures, such as nanotubes and nanowires, impose a tremendous challenge for experimental study of their mechanical properties and reliability. Although several micro/nanoscale tensile tests were used to mechanically characterize nanotubes and nanowires, the results were reported differently by different groups even on the same nanostructures. The critical issue that needs to be addressed is how to accurately measure nanoscale materials properties by tensile testing. We found out that the offset angle of sample alignment greatly affects tensile measurements at the micro/nanoscale. Tensile tests were performed on polyprypolene microfibers using a nanotensile tester. The engineering stress-strain curves were obtained from various alignment offset angle tests. The stress-strain distribution was analyzed by finite element analysis. The calibration technique for the offset angle has been developed.

2:50 PM
The Measurement of the Coefficient of Friction and Micromechanical Properties of Nanomaterials and MEMS: *Ethel Poiré*[1]; [1]Micro Photonics, Inc., 21 Morgan Ste. 100, Irvine, CA 92618 USA

Measuring the properties of nanomaterials and MEMS is especially challenging because of their size and fragility therefore requiring small loads for the evaluation of their mechanical properties. This paper will present instruments and techniques used to study the coefficient of friction of nanomaterials and devices/features in the sub-millimeter scale, as well as instruments used to characterize micro and nano mechanical properties such as hardness, Young's modulus and fracture.

3:10 PM Break

3:30 PM Invited
Fully Integrating Advanced Experimental Methods with Physics-Based Models at the Micro- and Nano-Scale: *David A. Johnson*[1]; [1]US Air Force Research Laboratory, Matls. & Mfg. Direct., Wright-Patterson AFB, Dayton, OH 45433 USA

Evaluation and calibration of sophisticated, physics-based models of material behavior are hampered by the relative paucity of data that is available through traditional test techniques. As an example, information available from a tension test typically consists of the applied load and strain averaged over a single area or relative displacement across two points of the specimen. This quantity of information may be sufficient for the simplest models, but physics-based models, which attempt to describe material behavior through understanding of the effect of material structure at every level, require a much greater amount of data. There are generally many degrees of freedom in these models, especially in multi-scale, nonlinear models, and the much greater amount of data is required to evaluate and calibrate these models. This leads to verified modeling and simulation, leading, in turn, to much better fundamental physical understanding of material behavior and finally to substantial cost avoidance in the entire materials-life-cycle. Modern experimental techniques offer great promise in acquiring these large amounts of data. In the case of a tension specimen, for example, full-field techniques can continuously determine the full two-dimensional and, in some cases, three-dimensional strain tensor for every point on the surface of the specimen's region of interest (ROI) throughout the duration of the test. This can be done at various size scales, and the resulting information is vital in calibrating and evaluating modern models of general, nonlinear, material behavior. Much attention has been focused on integrating modeling and experiments, but the emphasis has typically been on model development. It is the author's contention that, in the materials-behavior area, modeling efforts are typically far ahead of our ability to judge the efficacy and practicality of the models, and more attention should be focused on efficient and sophisticated experimental methods at all size scales, fully integrated with the modeling effort, to accomplish this judgment. Also, the tools that enable correlation between results from experiments and from models are relatively unsophisticated and need much greater development. As an example of this concept, results from the study of an advanced intermetallic material are presented. This material is in a fully lamellar form, with lamellar colonies grown to very large sizes by specialized heat treatment to facilitate study of the "microstructure." The large amount of data acquired through full-field techniques is vital in understanding the nonlinear behavior of this very complex material. Through this information, fundamental physical knowledge can be gained and then incorporated into the design system for this and similar materials. Such fundamental material-behavior information is vital to designers and modelers.

4:00 PM
In-Situ Mechanical Testing of Micron-Scale Structures in the Dual Beam FIB/SEM: *Robert Wheeler*[1]; Michael D. Uchic[2]; Daniel Sergison[3]; Frank J. Scheltens[1]; Dennis M. Dimiduk[2]; [1]UES, Inc., 4401 Dayton-Xenia Rd., Dayton, OH 45432 USA; [2]Air Force Research Laboratory, Matls. & Mfg. Direct., AFRL/MLLM, Wright Patterson AFB, OH 45433-7817 USA; [3]Sergison Machine, E. Peoria, IL USA

The Dual Beam Focused Ion Beam (FIB)-Scanning Electron Microscope (SEM) is currently being employed as a tool for the production of mechanical test specimens at the micron scale. This instrument uses a controlled Ga ion beam to "micro-machine" compression test samples with dimensions in the range of 1 to 50 microns in diameter. To date, testing of such samples has been performed outside the microscope using a commercial nanoindentation device. While this type of testing is highly satisfactory, the current test system does not allow one to view the sample during deformation. Direct imaging of the sample is highly desired, as not only can one make qualitative observations of the manner in which the microsamples deform, but readily-available displacement mapping methods potentially allow for highly-localized strain measurements. We have constructed a testing system that can function inside of an SEM or the Dual Beam microscope, which allows one to image the sample surface during compressive deformation. The system is equipped with a piezoelectric actuator for displacement-control testing, and a load cell for force measurement. Direct imaging of the sample is accomplished using the SEM or FIB columns. This talk will focus on the construction and application of this test system to testing metallic materials. In addition, this talk will also explore the extension of this test platform to tension testing.

4:20 PM
Application of Scanning Acoustic Microscopy in Characterizing LIGA Process Fabricated Micro-Gas Chromatograph Columns: *Abhinav Bhushan*[1]; *Vidyu Challa*[2]; Jim Mckeon[2]; Dawit Yemane[1]; Michael C. Murphy[3]; Jost Goettert[1]; Edward B. Overton[4]; [1]Louisiana State University, Ctr. for Advd. Microstruct. & Devices (CAMD), 6980 Jefferson Hwy., Baton Rouge, LA 70806 USA; [2]Sonix, Inc., 8700 Morrissette Dr., Springfield, VA 22152 USA; [3]Louisiana State University, Mechl. Engrg., 2508 CEBA, Baton Rouge, LA 70803 USA; [4]Louisiana State University, Dept. of Environ. Studies, 1285 Energy, Coast & Environ. Bldg., Baton Rouge, LA 70803 USA

This paper discusses the application of scanning acoustic microscopy (SAM) in characterizing LIGA fabricated nickel micro-gas chromatograph (GC) columns. These high aspect ratio columns provide volumetric gas flows equivalent to wider diameter columns thus enhancing the dynamic range of the columns without loss of resolution and minimize the pooling effect of the stationary phase during column coating. The columns were fabricated out of electroplated metal using the LIGA technique. A critical step in the process is to seal the open ends of the columns by electrodeposition. Any delamination at the nickel-nickel interface would be detrimental to sample analysis. SAM was used to non-destructively characterize the electroplated interface and thus the sealing efficiency of the fabrication process. Ultrasound waves reflect at material changes, and the reflected ultrasonic signal can be digitized to produce insightful images. Air is a total reflector of ultrasound, and shows up bright on images, making delaminations easy to detect.

4:40 PM
Estimated Hydrogen Concentration at the Crack Tip Region by Measuring the Lattice Dilation Using Neutron Diffraction Measurements for ASTM A710: *Guiru Liu Nash*[1]; Philip Nash[2]; Hahn Choo[3]; Luck L. Daemen[4]; Mark A.M. Bourke[4]; [1]GM, Electro-Motive Div., 9301 55th St., LaGrange, IL 60525 USA; [2]Illinois Institute of Technology, MMAE, 10 W. 32nd St., Chicago, IL 60616 USA; [3]University of Tennessee, Dept. of Matls. Sci. & Engrg., 319 Dougherty Hall, Knoxville, TN USA; [4]Los Alamos National Laboratory, LANSCE-12, Los Alamos, NM 87545 USA

The neutron diffraction technique has been used to measure lattice parameters in the crack tip region after hydrogen charging of HSLA ASTM A710 steel. It was found that the lattice parameter at the crack tip region increased with increasing charging time and applied load. The peak value of the lattice parameter was at approximately 3 mm from the crack tip. The maximum lattice parameter at the crack tip region was 0.28723 nm after 2 hours charging and under a constant loading condition of K=10 MPaÖm. Assuming the hydrogen atoms occupy the octahedral interstitial sites of a-Fe, a relationship between the lattice parameter and the hydrogen concentration has been found numerically. It was found that the hydrogen concentration at the crack tip could reach 1.3254´1027 atoms/m3 with a lattice parameter of 0.28727 nm. This large hydrogen concentration was due to hydrogen diffusion induced by the stress gradient at the crack tip region.

Applications of Orientation Microscopy Techniques to Phase Transformations: Ferrous Alloys II

Sponsored by: TMS - Materials Processing & Manufacturing Division, TMS - MPMD-Phase Transformations Committee-(Jt. ASM-MSCTS)
Program Organizers: Robert E. Hackenberg, Los Alamos National Laboratory, Materials Science and Technology Division, Los Alamos, NM 87545 USA; Richard W. Fonda, Naval Research Laboratory, Washington, DC 20375 USA; Milo V. Kral, University of Canterbury, Department of Mechanical Engineering, Christchurch New Zealand

Tuesday PM — Room: Mardi Gras Ballroom C
September 28, 2004 — Location: Marriott New Orleans Hotel

Session Chair: John J. Jonas, McGill University, Dept. of Matls. Engrg., Montreal, Quebec QC H3A 2B2 Canada

2:00 PM Invited
Application of Orientation Microscopy to Phase Transformations in Microalloyed Steels: *Guenter Gottstein*[1]; Ingo Lischewski[1]; [1]RWTH Aachen University, Inst. of Physl. Metall. & Metal Physics, Aachen 52056 Germany

Orientation microscopy by means of EBSD in a high resolution FEG-SEM offers the advantage of a local orientation measurement in very small volumes. By determination of the microstructure and local orientation before and after a phase transformation at the same location it is possible to establish a direct crystallographic correspondence between prior and subsequent phase. This can be utilized for an investigation into the mechanisms of phase transformations. We examined the diffusion controlled phase transformation from ferrite to austenite in a micro-alloyed steel. A special annealing treatment enabled a partial or complete stabilization of the high temperature phase (austenite). Pre- and post-transformation EBSD measurements at the same sample areas were conducted. The austenite was observed to nucleate at random triple junctions of pre-existing ferrite grain boundaries and the orientations of the nuclei satisfied the K-S (Kurdjumov-Sachs) orientation relationship. This is surprising, since the K-S relationship was actually derived for martensitic transformations. No apparent variant selection was observed during incipient stages of austenite nucleation. In contrast, with progressing phase transformation a marked variant selection occurred. The results substantiate that orientation microscopy can be utilized to obtain information on the orientation distribution, preferred nucleation sites and transformation mechanisms.

2:30 PM Invited
Orientation Microscopy Investigation of Phase Transformations in Low Carbon Steels: *George Spanos*[1]; C. R. Feng[1]; [1]Naval Research Laboratory, Physl. Metall. Branch, Code 6324NRL, 4555 Overlook Ave., SW, Washington, DC 20375-5000 USA

Orientation Microscopy/Electron Backscatter Diffraction (OM/EBSD) is employed here to study the evolution and crystallography of a relatively newly reported coarse autotempered martensite formed in low carbon alloy steels. OM/EBSD techniques are applied to differentiate (both qualitatively and quantitatively) between this coarse martensite and the coexisting fine lath martensite. This methodology is based on using the distributions of the EBSD diffraction pattern quality index (also referred to as "image quality" index), with emphasis on differentiating distributions of this index (and other EBSD indices) between various microconstituents in steels. Additionally, application of these techniques to other phase transformations in steels will be considered.

3:00 PM Invited
Rolling Texture and Proeutectoid Ferrite Growth Kinetics: *G. J. Shiflet*[1]; R. E. Hackenberg[2]; [1]University of Virginia, Dept. of Matls. Sci. & Engrg., 116 Engineer's Way, Charlottesville, VA 22904-4745 USA; [2]Los Alamos National Laboratory, Matls. Sci. & Tech. Div., MS G770, Los Alamos, NM 87545 USA

Fe-C binary steels have traditionally served as the model system for comparing experimental diffusional growth kinetics with theory. Because of several stereological difficulties that must be accounted for, either with statistical analysis or sample modification from the bulk, it is unclear whether new uncertainties are unintentionally added in. The presentation will reexamine ferrite growth kinetics in a high purity Fe-C steel heat treated isothermally in the ferrite + austenite phase field (above the Ae1) for a series of times. Samples for grain boundary ferrite growth kinetic measurement will include bulk ingots that have not been rolled or processed in any way beyond cutting the material into slices. These samples will be compared to material that is rolled from 50 to 90% obtaining the "bamboo" structure prior to heat treatment. Ferrite allotriomorph thickness will be determined by serial sectioning and computer reconstruction into three dimensional objects while orientation microscopy methods will highlight the effect of rolling on ferrite orientation distributions associated with different austenite grain boundaries.

3:30 PM Break

3:50 PM
Quantification of the Austenite to Ferrite Decomposition by EBSD: *Jinghui Wu*[1]; Peter J. Wray[1]; C. Isaac Garcia[1]; Anthony DeArdo[1]; [1]University of Pittsburgh, Dept. of Matls. Sci. & Engrg., 848 Benedum Hall, Pittsburgh, PA 15261 USA

The Electron Back-Scattered Diffraction (EBSD) technique is a relatively new and highly promising technique to study metallurgical reactions such as phase transformations. In this paper the application of EBSD to the quantitative analysis of the austenite to ferrite decomposition is presented and discussed. The complex mixture of austenite transformation products developed from three different steels: IF steel, Dual Phase steel and HSLA steel, were observed. The relative sharpness of EBSD patterns is normalized and used to quantify the volume fraction of the transformation products, especially the different types of ferrite observed. Image quality (IQ) maps and distributions have been carefully obtained, developed and compared by using a multi-peak distribution model. The influence of grain boundary effects on IQ resolution has been eliminated by using a data filtering software to minimize the errors in microstructural quantification. Compared with conventional methods of quantitative metallography, EBSD and IQ analysis has the potential to be an efficient and reliable technique to quantify the austenite decomposition products in steels.

4:15 PM
Investigation of the Bainitic Phase Transformation in a Low Alloyed TRIP Steel Using EBSD and TEM: *Stefan Zaefferer*[1]; [1]Max-Planck-Institute for Iron Research, Microstruct. Physics & Metal Forming, Max-Planck-Str. 1, Duesseldorf 40237 Germany

The formation of bainite in steels with transformation induced plasticity (TRIP) is of great importance to stabilize the austenite against too early martensitic transformation during straining. Austenite stabilization is achieved by a sufficient carbon supersaturation and by the mechanical stresses exerted by bainite formation. Understanding the structure and formation mechanisms of bainite is therefore necessary to optimise the TRIP effect. High resolution EBSD and TEM investigation revealed the following: Bainite consists of fine lamellae of ferrite and austenite which show a sharp Kurdjumov-Sachs orientation relationship with each other. This was interpreted in terms of a displacive bainite formation mechanism. It always occurs in conjunction with an orientation gradient in the surrounding ferrite matrix indicating the formation of shear stresses during transformation. The microstructure is formed by growth of g-grains during intercritical annealing and shrinking of these grains during the subsequent cooling without nucleation of new a-grains. The transformation first occurs reconstructively into ferrite and then, at lower temperature, displacively into bainite.

4:40 PM
EBSD Characterization of Cleavage Fracture in Pure Iron: *Raghavan Ayer*[1]; Russ Mueller[1]; [1]ExxonMobil Research and Engineering Company, Rm. LB242, 1545 Rte. 22 E., Annandale, NJ 08801 USA

Over recent years, Electron Backscattered Diffraction (EBSD) analysis has made significant inroads in crystal orientation, misorientation and phase analysis of materials. The present study describes the results of a study performed to characterize the crystallography of cleavage facets and sub surface twinning in pure iron. Cleavage fracture and twin traces of pure iron samples fractured in liquid nitrogen were examined by EBSD to determine the crystallographic details of the cleavage planes. The approach consisted of analyzing planes in orthogonal directions to achieve unique description of crystallographic indices as well as well as traces from several individual planes. The experimental methodology and results will be presented. The results will also be compared with cleavage fracture in commercial carbon steels.

Computational Microstructure Evolution in Steel: Multiphase Microstructure Evolution

Sponsored by: TMS - Structural Materials Division, TMS - EMPMD/SMD-Chemistry & Physics of Materials Committee, TMS - MPMD-Computational Materials Science & Engineering-(Jt. ASM-MSCTS)
Program Organizers: Koenraad G.F. Janssens, Sandia National Laboratories, Materials and Process Modeling, Albuquerque, NM 87185-1411 USA; Mark T. Lusk, Colorado School of Mines, Mechanical Engineering Program, Division of Engineering, Golden, CO 80401 USA

Tuesday PM Room: La Galerie 4
September 28, 2004 Location: Marriott New Orleans Hotel

Session Chair: Mark T. Lusk, Colorado School of Mines, Div. of Engrg., Golden, CO 80401 USA

2:00 PM Invited
PrecipiCalc(TM) Simulation of Alloy Carbide Precipitation in UHS Steels: *Greg B. Olson*[1]; H.-J. Jou[1]; [1]Northwestern University, Evanston, IL 60208 USA

Abstract not available.

2:40 PM
Mixed Microstructure Representation and Creation of Multi-Level Cellular Automata Objects: *Sumitesh Das*[1]; Partha Sarathi Mitra[1]; [1]Tata Steel, Automation Div., Jamshedpur, Jharkhand 831001 India

Certain regimes in thermo-mechanical processing of steels lead to the formation of mixed microstructures. Examples of these are: Ferrite grains in a austenite matrix, martensite in a ferrite matrix, precipitates of second phase in a austenite matrix. Some of these are specifically created to obtain desirable mechanical properties. For instance, the creation of martensite in ferrite either after hot rolling or annealing following cold rolling to acheive high strength dual phase steels. There is a need to understand the process of creating such microstructures as well as to obtain physcially based formulations for load calcualtions during deformation. The paper presents a methodology to capture the spatial variations of mixed microstructures and create Cellular Automata objects at appropriate length scales for integration with finite element codes of material deformation. The specific example addressed in this paper is that of martensite distribution in a ferrite matrix for a dual phase steel. The proposed strategy uses image processing techniques along with digitisation methods to capture the microstructure and delineate regions of influences. The algorithm is implemented on a Visual Basic platform and uses Ms-ACCESS as a database for data handling and cleaning. The automatic creation of Cellular Automata objects at different length scales provides an alternate method of representing spatial heterogenity commonly observed in mixed microstructures.

3:00 PM
Modelling of the Temporal Evolution of Particle Size Distributions in Crystalline Solids: *Johan Magnus Jeppsson*[1]; John Ågren[1]; [1]KTH, Matls. Sci. & Engrg., SE 100-44, Stockholm Sweden

In this talk we will present results obtained from a recently implemented model where nucleation and growth of precipitates are simulated. Nucleation is treated by means of classic nucleation theory and the temporal evolution of the size distribution is obtained by solving the Langer-Schwartz partial differential equation. All thermodynamic quantities, e.g. driving force for nucleation, are obtained from Calphad type of databases by means of a user interface to Thermo-Calc. Results presented include ferrite precipitation in austenite.

3:20 PM
Multi-Scale Modelling: Simulation of Deformed Austenite Decomposition into Ferrite During Phase Transformation: *Dianzhong Li*[1]; Yong-Jun Lan[1]; Ming-Ming Tong[1]; Na-Min Xiao[1]; Yiyi Li[1]; Chengjiang Huang[1];

[1]Chinese Academy of Sciences, Inst. of Metal Rsch., 72 Wenhua Rd., Shenyang 110016 China

This paper presents a multi-scale modeling for simulating deformed austenite decomposition into ferrite in low carbon steel, which is based on coupling thermo-mechanical finite element model (FEM) and crystal plasticity finite element model (CPFEM) with a probabilistic cellular automaton (CA). The multi-scale modeling links nucleation and growth kinetic models at the scale of sub-microns to the performance of products in meters. FEM accounts for macro-equivalent stress, strain and temperature evolution in deformation flat products, and CPFEM accounts for crystallographic slip and rotation of crystal lattice during plasticity deformation, the heterogeneity of stored energy is calculated. The information of stored energy, orientation angle of grains is translated into CA models. Based on the coupling of CPFEM and CA, potential nucleation sites will be identified both in grain boundaries and inner grains. The multi-scale modeling is applied to the simulation of inhomogeneous volume fraction and grain size in deformed flat.

3:40 PM Break

4:00 PM Invited

Effects of Austenite Grain Size on the Critical Temperatures and Kinetics of Bainitic and Martensitic Transformations in a Low Alloy Steel: *Young-Kook Lee*[1]; [1]Yonsei University, Dept. of Metall. Engrg., Seodaemun-gu, Seoul 120-749 Korea

Abstract not available.

4:40 PM

Phase Field Modelling of the Interfacial Condition at the Moving Interface During Austenite to Ferrite Transformation in C-Mn Steels: Maria Giuseppina Mecozzi[1]; *Jilt Sietsma*[1]; Sybrand van der Zwaag[2]; [1]Delft University of Technology, Dept. of Matls. Sci. & Engrg., Rotterdamseweg 137, Delft 2628AL The Netherlands; [2]Delft University of Technology, Faculty of Aeros. Engrg., Kluyverweg 1, Delft 2629HS The Netherlands

The phase field model is used in this paper to simulate the austenite to ferrite transformation in different cooling conditions. Since the effect of both a finite interface mobility and a limited carbon diffusion rate is considered, this model is an example of a mixed-mode model. It provides qualitative information on the developing microstructure, as well as a quantitative information on both the ferrite fraction formed and the carbon concentration distribution in the remaining austenite. The initial austenitic microstructure (grain morphology and dimensions) and the nucleation conditions (nucleus density and nucleation undercooling) are set as input data of the model; they are derived by metallographic and dilatometric tests. The interface mobility is the only parameter in the model that is hard to quantify from other sources. It is used as a fitting parameter to optimise the agreement between the experimental ferrite fraction curve, obtained by dilatometry, and the simulated ferrite fraction. A good agreement is obtained between the simulated microstructure and the actual microstructure observed after cooling. The derived carbon distribution in austenite also provides insight in the nature of the phase transformation with respect to the interface-controlled or diffusion-controlled mode. It is found that at the initial stage of the transformation is always nearly interface-controlled but gradually a shift towards diffusion control takes place.

5:00 PM

Experimental and Modelling Studies into High Temperature Phase Transformations: Dominic Joseph Phelan[1]; Mark Henry Reid[1]; *Rian Johannes Dippenaar*[1]; [1]University of Wollongong, Steel Inst., Northfields Ave., Wollongong, NSW 2500 Australia

Experimental and modelling studies have been conducted to probe high temperature phase transformations in Fe-C alloys. Novel experimental techniques have been developed for the in-situ study of solidification phenomena, in particular the peritectic transformation, using Laser Scanning Confocal Microscopy (LSCM). Experimental results have been used to benchmark simulations generated using Micress, a multi-component, multi-phase phase field-modelling package. The combination of in-situ experiments and modelling studies has led to new insights into the role of cooling rate and solute segregation on transformation kinetics.

5:20 PM

Application of the Johnson-Mehl-Avrami Equation to Numerical Predictions of the Pearlite Transformation: Garud B. Sridhar[1]; Alexandra Kulas[1]; Lisa Widodo[1]; Amanda Niazi[1]; *Eric M. Taleff*[1]; [1]University of Texas, Mechl. Engrg., 1 Univ. Sta., C2200, Austin, TX 78712-0292 USA

The classical description of eutectoid reaction progress using the Johnson-Mehl-Avrami (JMA) equation has been revisited for the development of a simple numerical technique to predict non-isothermal pearlite formation. An incubation time, t0, is used to calculate the onset of pearlite formation. Methods are established to extract the temperature-dependent incubation time and constants of the JMA equation (B and N) from isothermal transformation data, such as found in TTT diagrams. These derived values are applied in a numerical model to predict non-isothermal pearlite formation by using the additivity principle, which assumes step-wise isothermal behavior. The validity of this assumption in interrogated using experimental data.

Engineered Steel Surfaces: Corrosion Protection, Coatings, Scale

Sponsored by: AIST, TMS, AIST - Division VI, TMS - SMD-Corrosion and Environmental Effects Committee-(Jt. ASM-MSCTS)
Program Organizers: Bruce Kukuch, Ispat Inland Steel R&D, Coatings and Surface Technology, East Chicago, IN 46312 USA; Raúl B. Rebak, Lawrence Livermore National Laboratory, Livermore, CA 94550 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Tuesday PM — Room: Grand Ballroom L
September 28, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Bruce J. Kukuch, Ispat Inland Steel R&D, Coatings & Surface Tech., E. Chicago, IN 46312 USA; James Maloney, The Timken Company, Adv. Matls. R&D, Canton, OH 44706 USA

2:00 PM

An Investigation of the Effects of Si on the Adhesion Behaviour of the Reheating Scales in Low Carbon Steels: *Majid Baderestani*[1]; Abbass Zarei Hanzaki[1]; [1]Tehran University, Metall. & Matl. Dept., Tehran Iran

The formation of oxide scales during any reheating process in the rolling plants and their subsequent adhesion to the substrate has been of great industrial dilemma. In this study the effect of chemical composition and the interface roughness on the adhesion of oxide scale formed during reheating stage in three low carbon steels were investigated. The results indicated that by forming different spinel compounds in the scale/metal interfaces Si enhances the chemical bonding. In addition the latter increases the interface roughness, which in turn may result in a more severe mechanical bonding.

2:25 PM

Study of Surface Alloying of Steel During Hot Rolling: *P. C. Maity*[1]; [1]National Institute of Foundry and Forge Technology, Ranchi 834003 India

To improve the corrosion resistance of hot rolled low carbon steel long products, fine powders of FeCr, Al, FeCr + Al and FeSi were sprinkled on the surface of the hot rolled steel rods (900-1000°C) immediately before rolling. 15 mm rods were reduced to 7 mm in four stages in a groove rolling mill with intermediate soaking for 10 min. at 900°C. The alloy powders were sprinkled at each stage prior to rolling. The alloy powders were found to be bonded well over the surface. The corrosion resistance of steel surfaces coated/alloyed with Al and Al + Cr improved significantly in comparison to uncoated/unalloyed surface. Al reduces oxide scale over the surface and hence allows access of alloying elements to the metallic surface. Moreover, as the reduction of iron oxide by Al is exothermic, it assists in bonding and diffusion of alloying elements under roll pressure. Microstructure of the alloyed surface and interface as well as corrosion properties of the steel surface will be discussed.

2:50 PM

Nickel Surface Catalyst on Cold Rolled Steel Sheet for Improved Phosphatability and Corrosion Resistance: *Bruce Kukuch*[1]; John A. Rotole[1]; [1]Ispat Inland Research Laboratories, 3001 E. Columbus Dr., E. Chicago, IN 46312 USA

Nearly all cold rolled sheet steel undergoes phosphate pretreatment and paint application before being put into service. Corrosion protection is a key consideration during material selection for a given application. This paper presents the production sequence, analytical evaluation, and performance evaluation of a cold rolled sheet steel (CRS) bearing a surface catalyst that enhances phosphate formation and coverage during pretreatment, thereby significantly improving corrosion resistance after painting. The catalyst, elemental nickel, is incorporated into the surface of the CRS during a continuous cold rolling process, between continuous annealing and temper rolling. XPS and AES were used to characterize the composition, structure, and distribution of the nickel catalyst at the CRS surface. SEM was used to show the considerable improvements in zinc phosphate crystal size, shape, and coverage. Over the past 13 years, dozens of in plant, real-world paint line trials have demonstrated the consistent, usually very significant improvements in after painting adhesion and corrosion resistance. A beneficial side effect of the surface nickel catalyst is greatly enhanced corrosion resistance of the CRS before painting.

3:15 PM Break

3:25 PM
Microwave-Driven Pack Cementation Coating Process: *Terry Tiegs*[1]; James Kiggans[1]; G. Muralidharan[1]; [1]Oak Ridge National Laboratory, Metals & Ceram., PO Box 2008, MS 6087, Oak Ridge, TN 37831-6087 USA

Experiments were performed to determine if microwave heating can be used to apply diffusion coatings to metal alloy parts. Three metal alloys were selected: a tool steel (A2), a low carbon steel (1018), and a nickel-chrome super alloy (625). Three types of diffusion coating processes were chosen: aluminization, chromization, and boronization. Control samples were also processed by conventional heating for comparison. Aluminum, chrome, and boron based diffusion coatings were successfully created using microwave heating. These microwave-processed coatings show some similarities to the conventionally produced coatings, although significant differences also existed in some cases. Very encouraging results were obtained with the A2 tool steel processed using microwave heating.

3:50 PM
Effects of Silicon Content and Cooling Rate on the Solidification Microstructure of Al-Zn Alloys: *Ana Arizmendi Morquecho*[1]; A. Salinas[1]; F. Garcia[1]; E. Nava[1]; A. Maní[1]; R. Garza[1]; [1]Cinvestav-Saltillo Campus, Carr Saltillo-Mty km. 13, Ramos Arizpe 25900 Mexico

The microstructure of Al-43.5Zn-1.5Si coatings on steel strips is very sensitive to continuous hot dip processing conditions. The role of Si during formation of the coating is to control the metallurgical reactions between solid steel and liquid Al-Zn alloy. A very important parameter that influences the final coating microstructure is the cooling rate during solidification. The aim of this paper is to present the results of a thermal analysis experimental study on the effects that Si content (0.5-2.6wt%) has on the microstructure produced by solidification of Al-Zn alloys at cooling rates between 3 and 77ºC/s. It is shown that increasing the Si content over 1.6 wt% (the Si solubility limit in the Al-Si binary system) changes the solidification sequence and modifies the effects of cooling rate on SDAS, grain size, hardness and intermetallic compound chemical composition and morphology in the solidification microstructure of these alloys.

4:15 PM
Investigation of Corrosion Behavior and Microstructure of Zircaloy4 Irradiated by High Dose Ar and Kr Ion: *Qian Wan*[1]; Xinde Bai[1]; Xiaoyang Liu[1]; [1]Tsinghua University, Dept. of Matls. Sci. & Engrg., Beijing 100084 China

In order to investigate the ion irradiation effect on the corrosion behavior and microstructure of Zircaloy4, Zircaloy4 specimens were irradiated by Ar and Kr ion using an accelerator at an energy of 300 keV, with the dose from 1e15 to 1e17 ions/cm2. Post-irradiation corrosion tests were conducted to rank the corrosion resistance of the resulting specimens by Potentiodynamic Polarization Curve measurements. The vacancy profile induced by Ar ions irradiation was calculated using Monte Carlo simulation program SRIM 96, and measured by means of the slow positron annihilation spectroscopy (SPAS). The microstructures of the irradiated surface were examined using Glancing Angle X-ray Diffraction (GAXRD). The potentiodynamic tests showed that with the irradiation dose increasing, the passive current density decreased firstly and increased subsequently. The mechanism of the corrosion behavior transformation was due to the amorphous phase formation firstly and the recrystallization in the irradiated surface subsequently.

4:40 PM
Formation of Intermetallic Compounds in Al-43.5z-1.5Si Liquid Alloys: *Felipe de Jesús García Vásquez*[1]; A. Salinas[1]; A. Arizmendi[1]; E. Nava[1]; A. Maní[1]; R. Garza[1]; [1]Cinvestav-Unidad Saltillo, Carretera Monterrey-Saltillo Km. 13, Ramos Arizpe, Coahuila 25900 Mexico

Continuous hot dip Al-43.5z-1.5Si coating baths are permanently saturated with Fe as a result of their interaction with the solid steel strip. As result, any excess Fe in the liquid alloy leads to formation of solid AlSiFeZn intermetallic compound particles. These particles may be trapped in the coating overlay and leave the bath. However, more likely, they are redistributed and lead to dross accumulation at the bottom of the pot. In this paper it is shown that processing conditions, such a line velocity and bath chemical composition, have important effects on formation of AlFeSiZn intermetallic compounds. In addition, the results of an extensive chemical and microstructural characterization of the intermetallic compounds formed both in the liquid bath and at the steel-coating interface are presented. It is demonstrated that processing conditions also affect the morphology of the alloy layer at the steel-coating interface.

Intellectual Property Fundamentals for Materials Scientists and Managers: IP Fundamentals II: Asserting IP Rights

Sponsored by: TMS
Program Organizer: Steven P. Marsh, Frommer Lawrence & Haug LLP, New York, NY 10151 USA

Tuesday PM Room: Grand Ballroom I
September 28, 2004 Location: Marriott New Orleans Hotel

Session Chairs: Steven P. Marsh, Frommer Lawrence & Haug LLP, New York, NY 10151 USA; Edgar H. Haug, Frommer Lawrence & Haug LLP, New York, NY 10151 USA; Grace L. Pan, Frommer Lawrence & Haug LLP, New York, NY 10151 USA

2:00 PM Invited
Licensing and Agreements: Getting Value Out of Your IP: *Frommer Lawrence & Haug LLP*[1]; [1]745 Fifth Ave., New York, NY 10151 USA

Intellectual property, like other types of property, can be sold, but more often it is merely licensed. Anything from the manufacturing of patented inventions to the use of a designer's logo can be licensed, and licenses can be exclusive or non-exclusive. Licenses may be one of the more lucrative sources of income for companies. The components of typical licensing agreement will be presented in this talk, along with illustrations of how licenses have been used to create and leverage capital.

2:30 PM Invited
Technology Commercialization and Intellectual Property Management at Sandia National Laboratories: *Kevin A. McMahon*[1]; [1]Sandia National Laboratories, PO Box 5800, MS 0114, Albuquerque, NM 87185-0114 USA

Sandia National Laboratories (Sandia) actively seeks industrial commercialization partners (Partners) and manages intellectual property (IP) to ensure that such partnering is possible. Principles and practices by which Sandia conducts partnering and IP management, some of which are summarized below, are the basis of this presentation. A foremost goal is Research and Development (R&D) with Partners that contribute to Sandia's mission of developing and applying science and engineering solutions to national security. Sandia and a Partner may work together to jointly secure Federal funding for R&D projects. Agreement types include: Cooperative Research and Development Agreements, Work-for-Others and commercial licenses. Selection of type(s) depends on the nature of the technical project and the business interests of both parties. Sandia IP may be either created during an agreement with a specific Partner or created prior to such an agreement. Sandia licenses both types of IP ensuring the Partner has rights necessary for commercialization. Commercial licenses to Sandia IP include such terms and conditions as would be found in any commercial license agreement. Sandia IP is "born" with Government rights allowing for Government use.

3:00 PM Invited
Intellectual Property, Technology Transfer, and Qualification: The History of LENS™ Materials Processing Technology: *John E. Smugeresky*[1]; D. M. Keicher[2]; [1]Sandia National Laboratories, MS 9402/940-1191, 7011 East Ave., Livermore, CA 94551-0969 USA; [2]Optomec Design Company, 3911 Singer Blvd. NE, Albuquerque, NM 87109 USA

The model based Laser Engineered Net Shaping (LENS™) metal deposition process has emerged out of the ground work provided by the Rapid Prototyping community. Started as an internal R&D project, the technology evolved as a technical advance that constituted intelecctual property which Sandia protected through the patenting process. The LENS™ technology has since been developed as a mature enough technology to be licensed based on a patent and commercialized as a device for making net-shaped functional metal parts without molds or machining. A small business now produces several models of the device and the technology is being used in industry, government, and university applications. One of the most interesting uses is for doing materials research and development. This presentation will give the history of the development of the technology as an example of how intellectual property, patenting, and the entrepreneurial community can combine to tranform a laboratory curiosity into a money making business, without having to give up materials research. Work supported by the U. S. Department of Energy under contract DE-AC04-94AL85000. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy.

3:30 PM Break

3:45 PM Invited

The Business of Inventing New Materials: *Jainagesh A. Sekhar*[1]; [1]University of Cincinnati, Coll. of Engrg., 496 Rhodes Hall, Cincinnati, OH 45221-0012 USA

Over the past several years the intimate contact I have had with university IP, licensing, and company formation have provided me some insights into successful and unsuccessful outcomes. Some views on balancing the needs for publications and the need to protect ideas will be shared where it concerns research conducted at universities. A new tool, called the activity indicator, will be discussed for predicting the potential of inventions which deal with new material formulations.

4:15 PM Invited

IP Ownership Disputes: The Litigation Process: *Frommer Lawrence & Haug LLP*[1]; [1]745 Fifth Ave., New York, NY 10151 USA

In the world of business competition, it is inevitable that conflicts will result over one of a company's most valuable assets—intellectual property rights. A patent owner might discovery that someone is practicing his patented invention without authorization, or a company may be using another's distinctive name or signature packaging without authorization. When this happens, the IP owner has several options, and one of them may be to bring a suit against an alleged infringer. The stages of a typical litigation process will be outlined, including the initial filings, discovery, trial, and appeal. Alternatives to litigation, such as arbitration and monetary or licensing settlements, will also be discussed.

4:45 PM Invited

Participating in Litigation: Providing Expert Advice: *Frommer Lawrence & Haug LLP*[1]; [1]745 Fifth Ave., New York, NY 10151 USA

Scientists and engineers are often called in to participate in litigations by serving as expert witnesses. Depending on the case, an expert may be asked to testify, prepare expert opinion reports, or serve as a technical consultant for the litigation. This talk will discuss the range of duties of technical experts in each of these roles, along with some tips and guidelines on how to effectively work with counsel.

Materials Damage Prognosis: Probabilistics, Risk, and Uncertainty Methods I

Sponsored by: TMS - Structural Materials Division

Program Organizers: James M. Larsen, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson AFB, OH 45433-7817 USA; Jeffrey R. Calcaterra, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson Air Force Base, OH 45433-7817 USA; Leo Christodoulou, Defense Advanced Research Agency, Arlington, VA 22203-1714 USA; Michael L. Dent, Anteon Corporation USA; William J. Hardman, Naval Air Systems Command, Propulsion and Power Directorate (AIR 4.4.2), Patuxent River, MD 20670-1534 USA; Paul Hoffman, United States Navy, NAVAIR, Patuxent River, MD 20670 USA; J. Wayne Jones, University of Michigan, College of Engineering, Department of Materials, Science and Engineering, Ann Arbor, MI 48109 USA; Stephan M. Russ, Air Force Research Laboratory, Materials and Manufacturing Directorate, AFRL/MLLN, Wright-Patterson Air Force Base, OH 45433-7817 USA

Tuesday PM　　Room: La Galerie 5
September 28, 2004　　Location: Marriott New Orleans Hotel

Session Chairs: Jeffrey R. Calcaterra, Air Force Research Laboratory, Wright Patterson AFB, OH 45433 USA; Stephan M. Russ, Air Force Research Laboratory, Wright Patterson AFB, OH 45433 USA

2:00 PM Invited

Microstructural Modeling and Simulation for Prognostics: *Robert G. Tryon*[1]; Animesh Dey[1]; Yaowu Zhao[1]; Arun Iyer[1]; [1]VEXTEC, 750 Old Hickory Blvd., Bldg. 2 Ste. 270, Brentwood, TN 37027 USA

High strength components exposed to cyclic loading such as gas turbine disks fail in an insidious manner, giving no prior indication that damage has occurred. Cracking that takes place on a very small scale causes the disk failure. The critical damage state is reached when the crack is very small. Unfortunately, cracks of these sizes are difficult to detect. Often, long crack damage is considered when performing fatigue diagnostics. However, an accurate onboard prognostic capability should consider total life as initiation and long crack growth. Prognostication of small cracks requires simulating fatigue damage accumulation from the evolution of micro-scale damage initiation. VEXTEC has developed methods for predicting probability of fatigue failure. These methods predict the variation in fatigue life based on the statistical variation in the microstructure of the material. Material parameters at the metallic grain level are integrated with fundamental physics-based models to predict the damage as it accumulates.

2:25 PM Invited

Fatigue Crack Growth Variability in Waspaloy Under Representative Loading Conditions: *Michael J. Caton*[1]; Andrew H. Rosenberger[1]; James M. Larsen[1]; [1]U. S. Air Force Research Laboratory, Matls. & Mfg. Direct., AFRL/MLLMN, Wright-Patterson AFB, OH 45433-7817 USA

A key element of a material prognosis system is the ability to predict the variability in fatigue crack growth rates for given material systems and loading conditions. This study examines the variability in crack growth rates in Waspaloy at 650°C under several loading frequencies including the influence of dwell periods. Specimens were taken from different locations of several forged disks and the grain structures were characterized. It is observed that grain structure can vary significantly for different locations within single disks and from disk to disk. It is also observed that crack growth rates can vary by up to a factor of 5 for different specimens and that differences are generally more pronounced at lower frequencies and under dwell conditions where time dependent mechanisms are active. The role of microstructure in driving variability in crack growth rates and the implications for enhancing the physically-based models incorporated into materials prognosis systems will be discussed.

2:50 PM

The Role of Microstructure on Fatigue Life Variation in Alphpa/Beta Ti Alloys: *Alison K. Polasik*[1]; M. J. Mills[1]; J. M. Larsen[2]; H. L. Fraser[1]; [1]Ohio State University, Matls. Sci. & Engrg., 477 Watts Hall, 2041 Coll. Rd., Columbus, OH 43210-1179 USA; [2]Air Force Research Laboratory, Matls. & Mfg. Direct., AFRL/MLLMN, Wright-Patterson AFB, OH 45433-7817 USA

A crucial step towards the accelerated implementation of materials in aircraft engine components is to develop materials-specific, microstructurally-based models of fatigue. Within that goal, the focus of this work is to develop a more quantitative understanding of the impact of microstructural features on the fatigue behavior of $\alpha\beta$ titanium alloys. Previous work by Jha et al.[1] has demonstrated the existence of a bimodal distribution in fatigue lifetimes of $\alpha\beta$ -processed Ti-6246. A distribution between Type 1 (short-life) failures and Type 2 (long-life) failures was seen at lower stresses, with an order of magnitude difference between the lifetimes of the two failure regimes. The work presented focuses on identifying the microstructural differences between the two sample populations that account for this lifetime distribution. The investigation has employed extensive characterization techniques, including OIM, TEM and site-specific TEM foil extraction using the Focused Ion Beam. Additionally, fatigue tests are being performed on Ti-6246 with a colony microstructure, $\alpha\beta$ processed Ti-6Al-4V and colony Ti-64. These results will be compared to those for $\alpha\beta$ processed Ti-6246 to further explore the impact of microstructural features as well as alloy composition on fatigue lifetime variation. [1]Jha, S. K., Larsen, J. M., Rosenberger, A. H., and Hartman, G. A., Scripta Materialia, Vol. 48/12, June 2003, pp. 1637-1642.

3:15 PM Break

3:25 PM Invited

Multiscale Fatigue Modeling and Life Prediction for Al 7075-T651 Alloy: *Mark F. Horstemeyer*[1]; Yibin Anna Xue[1]; Brian Jordon[1]; [1]Mississippi State University, Ctr. for Advd. Vehicular Sys., Box 5405, Mississippi State, MS 39762 USA

Microstructure based multiscale fatigue modeling is applied to study the fatigue behavior of Al 7075-T651 alloys. The high cycle fatigue (HCF) life in this alloy is particularly sensitive to stress concentrations due to its widespread micron-size Si inclusions. First, the inclusion severity scales for crack formation were formulated in terms of the length-ratio of constrained microplasticity zone and the inclusions. Damage incubation and microscopic/physical small crack growth were simulated based on the model developed by McDowell, et. al. The strain lives under uniaxial, complete reversed loading for Al 7075 T651 were estimated for various severe particle sizes. The incubation life for small particles makes up over 50% of the total life in HCF regime but only about a small portion of the total life for relatively large particles. The interaction between particles was evaluated in the low cycle fatigue region. The undercertainty of the predicted fatigue life was estimated based on the randomness of particle size and its distribution.

3:50 PM Invited

MicroFaVa: A Micromechanical Code for Predicting Fatigue Life Variability: *Kwai S. Chan*[1]; Michael P. Enright[1]; Jong S. Kong[1]; [1]Southwest Research Institute, Matls. Engrg. Dept., 6220 Culebra Rd., San Antonio, TX 78238 USA

This paper summarizes the development of a probabilistic micromechanical code for treating variability in fatigue crack initiation and propagation lives resulting from microstructure variations. The code is based on a set of microstructure-based fatigue models that predict fatigue crack initiation life, fatigue crack growth life, fatigue limit, fatigue crack growth threshold, crack size at initiation, and fracture toughness. Using microstructure information as material input, the code is capable of predicting the average behavior and the confidence limits of the crack initiation and crack growth lives of structural alloys under LCF or HCF loading. Application of the model to predicting the effects of microstructure on the stress-life (S-N_f) and the fatigue crack growth response (da/dN versus ΔK) of Ti-6Al-4V will be presented to illustrate the utilities of the code for fatigue damage prognosis. Work supported by AFOSR through Contract No. F49620-01-1-0547, Dr. Craig S. Hartley, Program Manager.

4:15 PM Invited
Prediction of the Worst-Case Fatigue Failures of an Alpha+Beta Titanium Alloy: *Sushant K. Jha*[1]; James M. Larsen[2]; Charles Annis[3]; Andrew H. Rosenberger[2]; [1]Universal Technology Corp., 1270 N. Fairfield Rd., Dayton, OH 45459 USA; [2]Air Force Research Laboratory, AFRL/MLLMN, 2230, 10th St., Ste. 1, Wright Patterson AFB, OH 45433 USA; [3]Statistical Engineering, 36 Governers Ct., Palm Beach Gardens, FL 33418 USA

A mechanism-based life prediction based on expectation of the worst-case fatigue behavior is one of the keys to reducing the uncertainty in lifetimes. Our earlier work showed that the fatigue behavior of the a+b titanium alloy, Ti-6Al-2Sn-4Zr-6Mo (Ti-6-2-4-6) was composed of two superimposing failure mechanisms with divergent lives. This resulted in the apparent variability in lifetimes. The combined Cumulative Distribution Function (CDF) was modeled as superposition of individual failure modes. Here, we discuss the factors controlling the distribution in lives of the worst-case failure mode (i.e., the one having the lower mean life) and an approach to predict these failures. Lives of the worst-case failures were dominated by crack growth starting from the relevant microstructural unit size (which was the equiaxed primary a size in this material). A model to predict the worst-case failures was constructed. Each sample was considered to have a random fatigue threshold (i.e., a lower bound on its life). The probability density of the worst-case failure was then dependent on the distribution in the threshold. The threshold probability density can be determined experimentally or through simulation of the variation in crack growth given the relevant microstructural size scale.

4:40 PM
Sources of Uncertainty in Fatigue Cracking in the Superalloy IN100 Under Realistic Loading Conditions: *James M. Larsen*[1]; Andrew H. Rosenberger[1]; Michael Caton[1]; Kezhong Li[2]; W. J. Porter[2]; [1]Air Force Research Laboratory, Metals, Ceram., & NDE Div., 2230 Tenth St., Bldg. 655, Wright-Patterson AFB, OH 45433-7818 USA; [2]University of Dayton Research Institute, Dayton, OH USA

An essential element of an effective capability for material damage prognosis is a physically accurate model of the life-limiting damage processes. In many advanced structural systems, these damage processes involve fatigue crack initiation and growth to failure under cycle- and time-dependent conditions. Although there is much knowledge of these phenomena, and good empirical models exist, there is little basic information available to elucidate the materials-based uncertainties inherent in making life predictions. The current paper presents results on the superalloy IN100 in which highly efficient experimental methods have been used to quantify and understand sources of variability in fatigue cracking under a range of representative usage conditions. These findings are coupled with detailed quantitative microstructural characterization, and a microstructurally based model of uncertainties is presented in the context of a probabilistic lifing framework.

Materials Damage Prognosis: Probabilistics, Risk, and Uncertainty Methods II

Sponsored by: TMS - Structural Materials Division
Program Organizers: James M. Larsen, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson AFB, OH 45433-7817 USA; Jeffrey R. Calcaterra, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson Air Force Base, OH 45433-7817 USA; Leo Christodoulou, Defense Advanced Research Agency, Arlington, VA 22203-1714 USA; Michael L. Dent, Anteon Corporation USA; William J. Hardman, Naval Air Systems Command, Propulsion and Power Directorate (AIR 4.4.2), Patuxent River, MD 20670-1534 USA; Paul Hoffman, United States Navy, NAVAIR, Patuxent River, MD 20670 USA; J. Wayne Jones, University of Michigan, College of Engineering, Department of Materials, Science and Engineering, Ann Arbor, MI 48109 USA; Stephan M. Russ, Air Force Research Laboratory, Materials and Manufacturing Directorate, AFRL/MLLN, Wright-Patterson Air Force Base, OH 45433-7817 USA

Tuesday PM   Room: La Galerie 6
September 28, 2004   Location: Marriott New Orleans Hotel

Session Chairs: Andrew Rosenberger, Air Force Research Laboratory, Wright Patterson AFB, OH 45433 USA; Michael L. Dent, Anteon Corporation USA

2:00 PM Invited
Reasoning and Prediction Strategies for Prognosis: *Stephen Engel*[1]; David Hoitsma[1]; [1]Northrop Grumman Integrated Systems, Airborne Early Warning & Elect. Warfare, Bethpage, NY 11714 USA

The Structural Integrity Prognosis System (SIPS) is being developed in response to the need for better methods that permit the optimal use of DoD assets. Current methodologies recommend the retirement of most vehicles long before experience has shown this to be warranted. The primary source of this conservatism is uncertainty in the methods and tests used in current life prediction strategies. The SIPS approach reduces this uncertainty through the interactions of three integrated elements: multi-scale models, sensors and advanced reasoning and prediction strategies that recognize the stochastic nature of structural failures. SIPS relies on more accurate, physics-based models that embody the mechanics of isolated and coupled material failure modes. These models are tailored to individual vehicles initially through evaluation of micro-structural characteristics of the materials combined with an assessment of key initial-state parameters. Throughout the life of each vehicle, models are kept in agreement with vehicle health by interpreting data from sensors that measure the damaging forces experienced, and where practical, the material state itself. Each source of data and each model that uses these data involve uncertainty. This paper discusses reasoning strategies used to manage this uncertainty through better sensor interpretation, the fusion of information from sensors and models, and model/process adaptation. The paper also addresses prediction strategies used to make probabilistic assessments of future material state based on assessments of current state and models of future use.

2:25 PM
Diagnostics and Dynamic Loads Identification in a Metallic Thermal: *Douglas E. Adams*[1]; [1]Purdue University, Mechl. Engrg., Ray W. Herrick Labs., 140 S. Intramural Dr., W. Lafayette, IN 47907-2031 USA

Thermal Protection Systems (TPS) are critical structural components in future aero-vehicles in the United States Air Force programs. Thermal shock, acoustic loading and transient foreign object impact loading during launch and re-entry can cause degradation in the health of mechanically attached metallic TPS panels in the form of, for example, face sheet buckling, warping/cracking of standoff bolts or wrinkling to primary/secondary seals. To reduce turnaround times of such vehicles, the TPS must be quickly inspected and repaired using both pre-/post-flight Nondestructive Evaluation (NDE) and in-flight Structural Health Monitoring (SHM) technologies. In this work, simulated in-service transient loads are identified experimentally using physics-based models of the TPS and damage is identified experimentally in combined environments using passive mechanical acceleration transmissibility measurements on the back-side of the panel. It is demonstrated in simulations that certain types of damage are more apparent using SHM techniques during operation than traditional off-line NDE techniques due to the high thermal loads. Transmissibility functions are also shown in experiments to be effective at detecting and locating damaged standoff bolts in panels subjected to combined mechanical (~130 dB) and thermal loading (~200°F). Loads are also accurately identified using physics-based models of the panel and standoffs in conjunction with a direct parameter estimation method for experimental system identification.

2:50 PM
The Influence of Uncertainty in Usage and Sensor Feedback on Fatigue Damage Prognosis: *Stephen J. Hudak*[1]; Michael P. Enright[1]; R. Craig McClung[1]; Harry R. Millwater[2]; [1]Southwest Research Institute, Matls. Engrg. Dept., 6220 Culebra Rd., San Antonio, TX 78238 USA; [2]University of Texas, San Antonio, TX USA

Significant enhancements in the reliability and readiness of high value assets are believed to be possible through the development and implementation of prognosis systems based on data acquisition and data fusion from on-line sensors, combined with analytical methods for data interpretation and decision-making. This paper addresses two major sources of uncertainty in prognosis: usage uncertainty and sensing uncertainty. These sources of uncertainty are examined using a fully probabilistic, damage-based life prediction methodology. Although the underlying methodology is believed to be applicable to a wide range of components and structures, it is demonstrated for the specific case of a generic bladed compressor disc in an advanced military jet engine. Analyses are performed using the DARWIN® probabilistic life prediction code that was modified to perform crack initiation calculations (in addition to crack growth), and to accept actual engine sensor data from flight data recorders (FDRs). A method is presented for forecasting fatigue damage for various mission-planning scenarios. Statistical distributions of mission uncertainty are developed from FDR information for military fighter aircraft (F15/F100-PW-229) collected at four USAF bases over a period of three years (2001-2003). Analyses are also performed to demonstrate the significant reliability benefits of continuous monitoring of fatigue damage with onboard sensors versus periodic depot inspections. The trade-off between detection of early fatigue damage with relatively high uncertainty versus detection of damage later in life with less uncertainty is also examined. The overall results demonstrate the utility of integrating probabilistic damage assessments into the prognostics process, both for enhanced mission planning and reduction in sustainment cost.

3:15 PM Break

3:25 PM Invited
Prognosis for Gas Turbine Engine Bearings: *Michael James Roemer*[1]; Rolf F. Orsagh[1]; Jeremy Sheldon[1]; [1]Impact Technologies, 125 Tech Park Dr., Rochester, NY 14623 USA

A comprehensive engine bearing prognostic approach is presented in this paper that utilizes available sensor information on-board the aircraft such as rotor speed, vibration, lube system information and aircraft maneuvers to calculate remaining useful life for the engine bearings. Linking this sensed data with fatigue-based damage accumulation models based on a stochastic version of the Yu-Harris bearing life equations with projected engine operation conditions is implemented to provide the remaining useful life assessment. The combination of health monitoring data and model-based techniques provides a unique and knowledge rich capability that can be utilized throughout the bearing's entire life, using model-based estimates when no diagnostic indicators are present and using the monitored features such as oil debris and vibration at later stages when failure indications are detectable, thus reducing the uncertainty in model-based predictions. A description and initial implementation of this bearing prognostic approach is illustrated herein, using bearing test stand run-to-failure data and engine test cell data.

3:50 PM
Resolving Experimental Damage by Use of Uncertainty Analysis: Jim Ragsdale[1]; *Justin Jackson*[1]; Judy Schneider[1]; W. Glenn Steele[1]; [1]Mississippi State University, Mechl. Engrg. Dept., PO Box ME, Mississippi State, MS 39762 USA

Use of carbon fiber reinforced polymers (CFRP) by the aerospace industry for fuel tanks requires operation at extreme conditions. Cryogenic fuel tanks require the CFRP to operate well below the Tg of the polymer resulting in brittle behavior. Additional thermal strains induced by the CTE mismatch also have to be incorporated into the design. Initial attempts to use CFRPs on the X-33 program resulted in excessive leakage due to the formation of microcrack networks through the structural walls. Various methods are being proposed to toughen the polymer at cryogenic temperatures. We have devised a fixture to statistically validate the effect of polymer modifications on the susceptibility of the CFRP to microcrack under thermal and mechanical cyclic loading. As part of this screening program, an error analysis of the test apparatus incorporating uncertainty is used to validate the test differences. Results of the uncertainty analysis are used to evaluate the effectiveness of proposed resin modifications.

4:15 PM Invited
Addressing Uncertainty and Confidence in Prognosis: *George Vachtsevanos*[1]; [1]Georgia Institute of Technology, Sch. of Electl. & Computer Engrg., Atlanta, GA 30332-0250 USA

Long term prediction of the remaining useful life of a failing component/subsystem entails large-grain uncertainty and prognosis, therefore, must incorporate means to represent and possibly manage uncertainty. Moreover, in the execution of a mission, information regarding the confidence limit associated with the availability of a certain asset is crucial if the mission is to be completed successfully. An integrated prognosis architecture requires the development and implementation of "smart" algorithms that incorporate learning routines for prediction and uncertainty management. A data-driven Confidence Prediction Neural Network is introduced, therefore, that accommodates a learning scheme intended to "shrink" the uncertainty bounds, as more information becomes available. The architecture builds upon the Probabilistic Neural Network and General Regression Neural Network concepts. Both networks share a similar characteristic: lazy learning, i.e. learning processes are postponed from the training phase to whenever the networks are called upon to perform their specific functions. One important advantage of this lazy learning approach is that it requires almost no time for learning and another benefit is that it can classify clusters of data whose shapes may be irregular. The Confidence Prediction Neural Network employs a Parzen estimator as the confidence distribution function and, for a long prediction horizon, the confidence distribution spreads and grows over time by repetitively applying a one-step prediction technique. Thus, more prediction steps tend to increase the uncertainty associated with future predictions. Confidence distributions of several paths of the same prediction step are eventually combined to represent an overall confidence distribution. The final result of a time series prediction is a prediction tree where each branch in a time step is a set of actions. Learning to take appropriate actions means learning to emphasize correct actions and de-emphasize others. Thus, the learning rules chosen here support the structure of the Confidence Prediction Neural Network and render narrower confidence distributions. Finally, the prognostic curve (the output of prognostic routines) is modulated by a time-dependent distribution that provides the uncertainty bounds. An appropriate integral of such a distribution at each point in time results in the confidence level committed to completing the mission or, given a desired confidence level, the time to failure of a failing component. Appropriate performance metrics are briefly reviewed and the methodology is applied to a typical dynamic system for proof-of-concept purposes.

4:40 PM Invited
Application of Material Fatigue Modeling to Bearing Life Prognosis: *Sean Marble*[1]; [1]Sentient

Prognostics and Health Management systems diagnose current component states and project future condition to enable commanders and maintainers to make informed asset utilization or repair decisions. To accurately predict future component health, models of component degradation processes are needed. This presentation describes a physics-of-failure prognostic model for the initiation and propagation of bearing fatigue spalls. The model uses historic and estimated future operating conditions to determine future bearing condition and returns a probability density function of the bearing remaining useful life. The model, known as Contact Analysis for Bearing Prognostics or CABPro, uses first principles approaches such as damage mechanics to track material microstructure changes and eventual loss during the spall propagation phase. It takes into account material properties, bearing geometry, surface interaction, lubrication, and variable operating conditions. CABPro has demonstrated high predictive accuracy on tapered roller bearings and is currently being adapted for turbine engine bearings.

Mechanical Behavior of Body-Centered-Cubic (BCC) Metals and Alloys: Dynamic Behaviors

Sponsored by: TMS - Structural Materials Division, TMS - SMD-Mechanical Behavior of Materials-(Jt. ASM-MSCTS), TMS - SMD-Refractory Metals Committee, TMS - SMD-Structural Materials Committee

Program Organizers: George T. Gray III, Los Alamos National Laboratory, Dynamic Properties Team, Los Alamos, NM 87545-0001 USA; Thomas R. Bieler, Michigan State University, Department of Chemical Engineering and Materials Science, East Lansing, MI 48824-1226 USA; John J. Lewandowski, Case Western Reserve University, Department of Materials Science and Engineering, Cleveland, OH 44106 USA; Eric M. Taleff, University of Texas, Mechanical Engineering Department, Austin, TX 78712-1063 USA

Tuesday PM Room: Mardi Gras Ballroom A
September 28, 2004 Location: Marriott New Orleans Hotel

Session Chairs: George (Rusty) T. Gray III, Los Alamos National Laboratory, Matls. Sci., Los Alamos, NM 87545-0001 USA; Eric M. Taleff, University of Texas, Austin, TX 78712-0292 USA

2:00 PM
Defect Generation and Storage in BCC Metals Subjected to Shockwave Deformation: *George T. Gray, III*[1]; [1]Los Alamos National Laboratory, MST-8, MS G755, TA-3, Bldg. 1698, Los Alamos, NM 87545 USA

The role of mechanical properties and microstructural evolution are of the utmost importance in understanding a materials response to shock loading. Pure face-centered-cubic metals have been seen to exhibit enhanced flow stresses following shock prestraining compared to quasi-static loading. On the contrary body-centered-cubic (bcc) metals such as tantalum and Ta-10W alloy displayed no enhanced hardening. Pure iron however has shown varying responses depending on whether the peak shock pressure is below or above the alpha-to-epsilon, occurring at 13 GPa, shock-induced phase transition. Shock prestraining iron below 13 GPa was seen to induce no enhanced hardening. In this talk the role of the Pierels stress and Bauschinger effect in bcc metals and alloys on defect generation and storage in bcc-based metals and alloys subjected to shockwave doformation is discussed.

2:20 PM
Capturing the Anisotropy Evolution of Tantalum Using Real Time Imaging: *Carl P. Trujillo*[1]; George T. Gray, III[1]; Shuh-Rong Chen[1]; Reynaldo Chavez[1]; [1]Los Alamos National Laboratory, MST-8, MS G755, Los Alamos, NM 87545 USA

To capture the evolution of anisotropy in textured metals under high rate conditions, we developed a method that enables us to digitally resolve this event. Using a Taylor Anvil Test Facility, we dynamically deformed unalloyed Ta, whilst capturing real time digital images of the radial flow at the impact surface. We measured the elliptical footprint and plotted its eccentricity (ratio of major to minor diameters) versus real time. The current engineering strength constitutive models allow for an initial texture, but they cannot accurately predict the texture evolution during deformation. This test will allow us to track anisotropy to better validate our constitutive models.

2:40 PM
Nano-Scale Twinning and Martensitic Transformation in BCC Metals Deformed Under Dynamic Pressures: *Luke L. Hsiung*[1]; [1]Lawrence Livermore National Laboratory, Chmst. & Matls. Sci., 7000 East Ave., L-352, PO Box 808, Livermore, CA 94551-9900 USA

Shock-induced twinning and martensitic transformation in BCC metals and alloys (Ta, Ta-W, and U6Nb) have been investigated using transmission electron microscopy(TEM). The length-scale of domain thickness for both twin lamella and martensite phase is smaller than 100 nm. While deformation twinning of {112}<111>-type is found within Ta when shock-deformed at 15 GPa, martensitic transformation is found when shock-deformed at 45 GPa. Similar phenomena of twinning and martensitic transformation are also found within U6Nb. Since both deformation twinning and martensitic transformation occurred along the {211}b planes associated with high resolved shear stresses, it is suggested that both can be viewed as shear transformations occurred in shocked BCC metals. Dynamic dislocation mechanisms for the shock-induced shear transformations are accordingly proposed. This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

3:00 PM
The Mechanical Response of Tantalum Loaded Dynamically in Shear: *Ellen Cerreta*[1]; George T. Gray[1]; Carl M. Cady[1]; [1]Los Alamos National Laboratory, MST-8, MS G755, Los Alamos, NM 87545 USA

Shear localization is often a dominant failure mechanism at high strain rates in ductile materials. While the constitutive behavior of tantalum has been established through a series of quasi-static and dynamic compression experiments over a range of temperatures, the development of the microstructure and substructure under high strain rate shear loading conditions remains poorly understood. The purpose of this study is to characterize the mechanical response and the deformation microstructure of as-annealed, cold rolled, and shock prestrained tantalum under dynamic shear loading conditions and to understand the mechanisms for shear deformation with in tantalum.

3:20 PM Break

3:40 PM
The Development of a Physically Based Constitutive Damage Model for a Cabot Tantalum: *William Richards Thissell*[1]; Davis L. Tonks[2]; Daniel S. Schwartz[3]; [1]Los Alamos National Laboratory, MST-08, G755, MST-08 G755, Los Alamos, NM 87545 USA; [2]Los Alamos National Laboratory, X-7: Matls. Modlg., F699, Los Alamos, NM 87545 USA; [3]Los Alamos National Laboratory, NMT-16: Plutonium Metall., G721, Los Alamos, NM 87545 USA

A suite of gas-gun propelled flyer plate experiments that were momentum trapped and soft recovered were performed on a Cabot Tantalum. The shock duration and amplitude were varied to cover a range of incipient damage states from low porosity to levels close to the percolation threshold for failure surface formation. The resulting samples were sectioned and metallographically prepared. Optical microscopy and optical profilometry was used to obtain complete composite information of all of the damage features that intersect two section planes. This information is quantified, distilled, and statistically reduced to produce porosity distributions, volumetric void number density distributions, expected size distributions, clustering and neighbor distance information, and deformation band area and size distributions of each experiment. This information is used to develop, validate, and calibrate a constitutive damage model through the process of simulation of experiments for use in explicit finite element simulations of structural performance.

4:00 PM
A Model for the High-Strain-Rate Response of BCC Metals: *K. T. Ramesh*[1]; [1]Johns Hopkins University, Mechl. Engrg., 3400 N. Charles St., Baltimore, MD 21218 USA

A high-strain-rate constitutive response function based on kink-dominated dislocation mobility is constructed for bcc metals, with the high-stress response determined by appeal to recent atomistic results by other researchers. The result is a constitutive model that is applicable over a wide range of strain rates at low homologous temperatures. Next, a suite of experimental techniques is described for the determination of these material properties at high rates of deformation, and the predictions of the model are compared with recent experimental observations of the mechanical behaviors of nanostructured iron, vanadium and tantalum over a wide range of strain rates.

4:20 PM
Mechanical Properties and Constitutive Modeling for BCC Metals: *Shuh Rong Chen*[1]; George T. (Rusty) Gray, III[1]; [1]Los Alamos National Laboratory, Matls. Sci. & Tech., MS G755, Los Alamos, NM 87545 USA

The high density and high melting temperature of several refractory metals make them attractive candidates for defense applications. The mechanical properties of these metals are very sensitive to deformation temperature, strain rate, and the impurity contents due to its more open crystallographic structure (bcc) with a higher intrinsic barrier (Peierls stress) to dislocation movement. In this talk, we will present constitutive properties on Ta, Mo, W, and their alloys obtained by compressing samples as a function of temperature from 77 to 1273K, and strain rate from 0.001/s to 3000/s. We will also present the development of more physically-based constitutive models to describe the mechanical responses of these metals to large strains. And finally we will validate the models and their corresponding parameters using high velocity Taylor cylinder impact tests by comparing results from the post-mortem plastic deformation profiles and the finite element calculations. Work supported jointly by the U.S. Department of Energy and Department of Defense.

4:40 PM
The Effects of Surface Condition and Initial Flaw Size on Dynamic Failure of Tungsten Heavy Alloy: *Kenneth R. Tarcza*[1]; Eric M. Taleff[1]; Stephan Bless[2]; [1]University of Texas, Mechl. Engrg., 1 Univ. Sta., C2200, Austin, TX 78712-0292 USA; [2]University of Texas, Inst. for Advd. Tech., Austin, TX 78759-5316 USA

The dynamic failure of tungsten heavy alloy (WHA) has been investigated using two types of mechanical tests. Experiments using a drop tower tested for dynamic failure behaviors at moderate strain rates and reverse-ballistic experiments in a light-gas gun tested for dynamic failure behaviors at hypervelocity rates. Two WHA compositions were tested, one with an Fe-Ni matrix and the other with an Fe-Co matrix. Test specimens were prepared by electrical discharge machining (EDM), which induces surface cracks that penetrate the specimen to approximately one grain diameter. Centerless grinding and polishing were applied to reduce surface roughness and initial flaw size. Improved surface finishes, with corresponding reductions in initial flaw size, resulted in increased fracture energies during drop-tower experiments. In reverse-ballistic experiments, improved surface finish transitioned failure from segmented fracturing to fragmentation.

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Mechanical Behavior of BMG/BCC Metal Composites: Paul Wesseling[1]; Awlah Awadallah[1]; John J. Lewandowski[2]; [1]Case Western Reserve University, Dept. Matls. Sci. & Engrg., Cleveland, OH 44106 USA; [2]Cambridge University, Dept. Matls. Sci. & Metall., Cambridge CB2 3QZ UK

The mechancial behavior of bulk metallic glasses (BMG) can be significantly altered via composite approaches. The effects of the addition of BCC metals on the deformation, fracture, and fatigue behavior of BMG/BCC metal composites is being determined under a range of different stress states and test temperatures. The effects of changes in testing conditions on the flow and fracture behavior have been determined with and without the superposition of hydrostatic pressure, while changes in test temperature have been used to change the flow and fracture behavior of the BCC metal. The effects of such changes to the flow and fracture of the BMG/BCC metal composites will be reviewed.

Modeling and Computer Applications in Metal Casting, Shaping & Forming Processes: Modeling and Computer Applications: Casting Processes

Sponsored by: AIST, TMS - Extraction & Processing Division, TMS - Materials Processing & Manufacturing Division, TMS, TMS - MPMD/EPD-Process Modeling Analysis & Control Committee, TMS - MPMD-Shaping and Forming Committee, TMS - MPMD-Solidification Committee, AIST - Division VI, AIST - Division VII, TMS - MPMD-Computational Materials Science & Engineering-(Jt. ASM-MSCTS)

Program Organizers: Krich Sawamiphakdi, The Timken Company, R&D Manufacturing Technology, Canton, OH 44706 USA; Praveen Pauskar, The Timken Company, Advanced Process Technology, Timken Research, Canton, OH USA; Maciej Pietrzyk, Akademia Gorniczo-Hutnicza, Department of Computer Methods in Metallurgy, Krakow Poland; Raghavan Srinivasan, Wright State University, Department of Mechanical & Materials Engineering, Dayton, OH 45435 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA; Brian G. Thomas, University of Illinois, Department of Mechanical and Industrial Engineering, Urbana, IL 61801 USA

Tuesday PM Room: La Galerie 2
September 28, 2004 Location: Marriott New Orleans Hotel

Session Chair: Brian G. Thomas, University of Illinois, Mechl. & Indust. Engrg. Dept., Urbana, IL 61801 USA

2:00 PM

Effects of Process Variables and Size-Scale on Solidification Microstructure in Laser Deposited Ti-6Al-4V: Nathan W. Klingbeil[1]; *Srikanth Bontha*[1]; Deepika Gaddam[1]; [1]Wright State University, Mechl. & Matls. Engrg., 209 Russ Engrg., 3640 Colonel Glenn Hwy., Dayton, OH 45435 USA

This work employs simulation-based methods to relate deposition process variables (laser power and velocity) to resulting microstructure (grain size and morphology) in laser deposited Ti-6Al-4V. Based on the Rosenthal solution for a moving point heat source, dimensionless process maps are presented for solidification cooling rate and thermal gradient over a wide range of laser deposition process variables. Results for both small-scale (LENS™) and large-scale (higher power) processes are plotted on solidification maps for predicting grain morphology in Ti-6Al-4V. The effects of temperature-dependent properties and latent heat are further included through thermal finite element modeling. Finally, results from 3-D cellular automaton solidification modeling are used to provide direct predictions of solidification microstructure in Ti-6Al-4V, and results are compared to both soldification map predictions and experimental observations. Results suggest that changes in process variables and size-scale can have a significant effect on solidification microstructure in Ti-6Al-4V.

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Modeling and Experimental Investigation of Spray-Formed H13 Steel Tooling: *Yaojin Lin*[1]; Young-Soo Park[1]; Yinghang Zhou[1]; Kevin M. McHugh[2]; Enrique J. Lavernia[1]; [1]University of California, Dept. of Chem. Engrg. & Matls. Sci., Davis, CA 95616-5294 USA; [2]Idaho National Engineering and Environmental Laboratory, Indust. & Matl. Tech. Dept., Idaho Falls, ID 83415 USA

Aimed at materials scientists and engineers, this paper is associated with a novel technique to fabricate molds and dies, "spray-formed tooling". Rapid cooling during spray-formed tooling may suppress carbide precipitation and allow tool steels to be artificially aged. In this paper, a numerical model is developed to calculate the cooling rates of H13 steel during spray-formed tooling. The critical cooling rate to suppress carbide precipitation is predicted. Microstructure and hardness of as spray-formed tooled H13 are investigated.

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Numerical Modeling of the Stresses and Strains in Bloom During Continuous Casting: *Andre Milenin*[1]; Henryk Dyja[1]; [1]Czestochowa University of Technology, Faculty of Process & Matls. Engrg. & Applied Physics, Al. Armii Krajowej 19, Czêstochowa 42-200 Poland

The paper considers the task of numerical modeling and optimization of the stresses and strains in the metal cast in the machine of continuous casting of blooms. The coupled model consisted of the phenomena of the heat exchange, solidification, thermal stress occurrence and relaxation, bloom bending and unbending is developed. The solution is obtained by using the finite element method. Researches on the influence of roller locations in the bending and unbending zones on the stresses and strains in the bloom are completed. To obtain the mechanical properties of the metal at high temperatures, plastometric and dilatometric tests are fulfilled.

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Molten Pool Size in Laser Cladding Simulated by Finite Element Method: Zhiyong Hu[1]; Guofang Zhou[1]; *Philip G. Nash*[1]; Calvin Tszeng[1]; [1]Illinois Institute of Technology, Thermal Procg. Tech. Ctr., 10 W 32nd St., Mechl., Matls. & Aeros. Engrg., Chicago, IL 60616 USA

Laser cladding is a process to add a layer of material onto a substrate to improve surface properties or to increase the dimensions. The phenomena in the molten pool during the process are very complicated making it difficult to consider all the factors influencing the process. We have used finite element method to investigate the temperature field for this case. In the temperature field we can easily find the size of the heat affected zone, and the size of the molten pool. We use the same parameters to perform the experiments using IR thermography and thermocouples to monitor the temperature field during the experiments. In this paper, we use Cu70-Ni30 for the cladding and substrate. Using microscopy we can easily determine the shape and size of the molten pool. The experiments validate the simulation results. From this validation, we can change the parameters to control the laser cladding process.

3:50 PM

The Importance of Metal-Mold Interface Heat Transfer Modeling in Solidification Simulation: *Prasanna Kumar Sanjivachar Thupaki*[1]; [1]Indian Institute of Technology, Dept. of Metallurgl. & Matls. Engrg., Chennai, TN 600036 India

The ability to predict and control morphology of castings through solidification simulation depends upon the modeling of heat transfer at the metal/ mold interface. Since the solidification is a dynamic process governed by the rate at which heat transfer takes place at the metal/mold interface, the boundary condition to be applied at the metal mold interface becomes critical. Several quantitative models to predict heat transfer coefficient have been developed using experimental data involving unidirectional solidification with casting and chill as a interface. Number of variables such as chill thickness, chill material, surface roughness etc. is considered. Such an approach has only limited application to a particular casting/mold configuration. A general model, which is applicable to all systems, is still not available. There is a need for evolving a method, which must be able to address the actual process parameters governing the metal/mold interface heat transfer. A convenient albeit artificial way of quantifying the heat transfer at the metal/mold interface is to define a heat transfer coefficient defined as the ratio of the heat flux and the local temperature difference between the casting and the mold surfaces. The goal of this article is to compare the efficacy of modeling (a) heat transfer coefficient and (b) heat flux at the metal-mold interface for solidification simulation. To use the heat transfer coefficient model effectively, we are required to compute the mold side temperature as well, which means that we should include the mold also in our calculation domain. On the other hand, the heat flux model has the advantage that the mold can be excluded form the calculation domain resulting in less CPU time and hence lower cost of simulation. The methodologies involved in developing these models are critically examined in this paper, for several casting processes. The interface heat transfer is generally modeled based on temperature measurements inside the mold wall and obtaining the heat transfer coefficient by theoretical calculations. It is generally limited to the simplest case of 1-D heat transfer. However, it is known that the solidification behavior of castings at the corners is substantially different from that at the middle of a plate. The heat transfer rate can be different at different locations within the casting, say from the corner to the middle of a plate like casting. To address this issue specifically, a new algorithm has been developed which is capable of delineating multiple components of the heat flux at the boundary using simple temperature measurements inside the mold. The new algorithm will help in quantifying the interface heat transfer more accurately so that the results of simulation are more realistic at the same time reducing the cost of simulation.

4:15 PM
The Helium Effect on the Simulation of Permanent Mold Casting Process: *Xianhua Wan*[1]; [1]University of Michigan, Matls. Sci. & Tech., 2300 Hayward St., Ann Arbor, MI 48109-2136 USA

During the permanent mold casting process, the metal/mold interfacial heat transfer coefficient (IHTC) is a key factor in determining the cooling rate of the casting. It is known that the simultaneous expansion of the mold and contraction of the solidifying casting leads to the formation of a gap which can have a large impact on the IHTC. It has been found that the primary mechanism of heat transfer across the gap in permanent mold casting is by conduction which in current standard practices would contain air. This paper will present that helium, a gas with thermal conductivity approximately six times higher than that of air, will significantly increase the heat transfer rates and reduce the cooling times. The helium effect on the simulation of permanent mold casting process has been explored. Comparisons have been made between the computer modeling and experiments. The economic benefits from helium injection are summarized.

4:40 PM
Investigation of Computational Issues in Modeling Turbulent Flow During Continuous Steel Casting: *Quan Yuan*[1]; *Brian G. Thomas*[1]; S. P. Vanka[1]; [1]University of Illinois, Dept. of Mechl. Engrg., 120 W. Green St., Urbana, IL 60801 USA

Unsteady three-dimensional turbulent flow in the nozzle and mold regions of continuous steel casters has been computed using different turbulent models, domains, grids, and inlet conditions. Comparisons are made between results from large eddy simulations (LES) and Reynolds averaged approaches (k-e model). Computational issues such as the selection of appropriate grid resolutions and Sub-Grid Scale (SGS) turbulence models (for LES) are investigated.

5:05 PM
Formation of the Dispersed Microstructure in a Strip Cast Immiscible Alloy: *J. Z. Zhao*[1]; L. Ratke[2]; [1]Chinese Academy of Sciences, Inst. of Metal Rsch., Shenyang China; [2]Institute for Space Simulation, DLR, Koln Germany

Immiscible alloys are a broad kind of materials. Many of them have great potentials to be used in industry if a finely dispersed microstructure can be obtained. These alloys, however, have an essential drawback that just the miscibility gap in the liquid state poses problems during solidifications. Under general solidification conditions, the components of alloys separate quickly during cooling in the miscibility gap and the microstructure with severe segregation is obtained. Strip casting may have potentials in the manufacturing of immiscible alloys. Experiments have been carried out with Al-Pb based alloys. A model has been developed to describe the microstructure evolution in a strip cast immiscible alloy. The formation of the microstructure has been explained in detail with this model.

Pb-Free and Pb-Bearing Solders: Session IV

Sponsored by: Electronic, Magnetic & Photonic Materials Division, EMPMD-Electronic Packaging and Interconnection Materials Committee
Program Organizers: C. Robert Kao, National Central University, Department of Chemical and Materials Engineering, Chungli City 32054 Taiwan; W. Plumbridge, Open University, School of Engineering Materials, Milton Keynes MK7 6AA UK; K. N. Subramanian, Michigan State University, Chemical Engineering & Material Science, East Lansing, MI 48824 USA

Tuesday PM Room: Grand Ballroom K
September 28, 2004 Location: Marriott New Orleans Hotel

Session Chairs: Eric J. Cotts, Binghamton University, Dept. Physics & Matls. Sci., Binghamton, NY 13902-6000 USA; J. K. Shang, University of Illinois, Dept. of Matls. Sci. & Engrg., Urbana, IL 61801 USA

2:00 PM Invited
Atomic Radius Effect on Intermetallic Coarsening in Thermal Aging of Tin-Silver-Copper-X Solder Joints: *Iver Eric Anderson*[1]; Joel L. Harringa[2]; Bruce A. Cook[2]; [1]Iowa State University, Ames Lab., Matls. & Engrg. Physics Prog., 222 Metals Dvlp. Bldg., Ames, IA 50011 USA; [2]Iowa State University, Ames Lab., MEP Prog., 47 Wilhelm Hall, Ames, IA 50011 USA

Since many new Pb-free electronic assembly applications involve service at high temperature and stress levels, promising Sn-Ag-Cu (SAC) solder alloys require microstructural stability on high temperature aging to retain joints with both strength and ductility. Recent work demonstrated the strategy of modifying a strong (high Cu) SAC solder alloy with a substitutional alloy addition (X=Co, Fe) for Cu to achieve this purpose. New work involves an expanded series of smaller and larger substitutional elements, e.g., Ni, Si, Ge, Ti, Cr, to a SAC+X solder, studying joint microstructures (pure Cu substrates) and shear strength after isothermal aging at 150°C for time intervals out to 1,000 hrs. Microanalytical electron probes will track phase coarsening and determine the role of local segregation on suppressing diffusion and embrittlement. Project funding received from Iowa State University Research Foundation with additional support from USDOE-BES through contract no.W-7405-Eng-82.

2:30 PM Invited
Bismuth Segregation at Sn-Cu Reactive Interfaces: *J. K. Shang*[1]; P. L. Liu[1]; C. Z. Liu[2]; [1]University of Illinois, Dept. of Matls. Sci. & Engrg., 1304 W. Green St., Urbana, IL 61801 USA; [2]Inst. of Metal Rsch., Shenyang Natl. Lab. for Matls. Sci., Shenyang 110016 China

Bismuth redistribution was examined in Cu/Sn-Bi interconnects to investigate the roles of alloying element in influencing structure and properties of Sn-Cu reactive interface. In-situ Auger fracture studies showed that Bi tends to segregate to Cu/intermetallic interface upon isothermal aging at different temperatures following the reflow. In the early stage of the interfacial segregation, accumulation of the segregants led to monolayer coverage of the interface, resulting in slower intermetallic growth and brittle fracture at the reactive interface. Upon further aging, the segregants evolved into particles. As a result, the kinetics of intermetallic growth was restored but the interfacial cavities were created. The roles of interfacial segregants will be discussed on the basis of a vacancy condensation model.

3:00 PM
Control of Interfacial Embrittlement in Pb-Free Solder Interconnects by Interfacial Alloying: *P. L. Liu*[1]; J. K. Shang[1]; [1]University of Illinois, Dept. of Matls. Sci. & Engrg., 1304 W. Green St., Urbana, IL 61801 USA

Bismuth was recently found to segregate to the reactive Sn-Cu interface and cause severe interfacial embrittlement. In this study, interfacial alloying was investigated as a potential method to mitigate the deleterious effect of Bi on mechanical properties of Sn-Cu interface. Alloying elements were introduced to both the solder and the metallization to create complex intermetallic compounds at the interface. While some of the alloy elements were not effective in inhibiting Bi-segregation, others were found to greatly reduce the embrittlement tendency of Bi-containing solder interconnects. The effects of the alloying elements are discussed on the basis of chemical modifications in the intermetallic compounds.

3:25 PM
Causes of Surface Topography (Pre-Damage) Development in Lead-Free Solder Joints: *Adwait U. Telang*[1]; Thomas R. Bieler[1]; [1]Michigan State University, Chem. Engrg. & Matls. Sci., 2527 Engrg. Bldg., E. Lansing, MI 48824 USA

The deformation in lead-free solder joints is very heterogeneous and sensitive to strain and temperature history. Surface topography develops in lead-free solder interconnects tested under different conditions in several different specimen geometries. Single shear lap specimens were subjected

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to creep, isothermal aging and thermomechanical fatigue (TMF) testing and observed using SEM and Orientation Imaging Microscopy (OIM). Dual shear specimens with different stress histories were also tested with TMF. Prior studies using OIM have shown that solder joints are typically multicrystals. SEM micrographs of previously polished specimens revealed changes in surface topography after creep and TMF. Ledges and grain boundary sliding have been frequently observed, correlating with both low and high angle grain boundaries, indicating a close relationship between deformation mechanisms and grain boundaries in tin-based joints. However, in joints where almost a single crystal was present (or developed during aging or TMF), the surface topography also revealed shear band features in grain interiors as well as ledges along certain grain boundaries. These shear band features frequently correlate with {110} plane traces. The underlying causes for these different surface damage features in grain interiors vs. grain boundaries will be addressed to examine how damage accumulation occurs in lead-free solder interconnects.

3:50 PM Break

4:05 PM Invited
Solidification and Deformation Behavior of SnCuAg Alloys: *Eric J. Cotts*[1]; Lawrence P. Lehman[1]; [1]Binghamton University, Physics & Matls. Sci., Sci. Two, PO Box 6000, Binghamton, NY 13902-6000 USA

We have examined the solidification and deformation behavior of Sn-Cu-Ag alloys of near the eutectic composition. In these alloys, both Ag3Sn and Cu6Sn5 intermetallic compounds can nucleate and grow with minimal undercooling, while the Sn matrix displays marked undercooling. Thus the protracted growth of one or both the compounds in the melt may be allowed. Furthermore, after the ultimate nucleation of Sn, its growth is rapid, and relatively large (mm) size dendritic crystals are observed. Microstructures were examined using electron and optical microscopy, with the ultimate goal of understanding the processes which control the evolution of these microstructures. The birefringent properties of Sn allowed delineation of Sn grains by means of optical microscopy in as cast, and in deformed samples. Correlations between crack formation and grain boundary locations were observed and studied for a number of deformation geometries. Support from the National Science Foundation, DM0218129 is gratefully acknowledged.

4:35 PM Invited
Solidification of the Sn-Ag-Cu-Ni Quaternary Alloys: Cheng-an Chang[1]; *Sinn-wen Chen*[1]; Cheng-nan Chiu[1]; Yu-chih Huang[1]; [1]National Tsing Hua University, Chem. Engrg. Dept., #101, Sec. 2, Kuang-Fu Rd., Hsin-Chu 300 Taiwan

Sn-Ag-Cu solders are the most promising lead-free solders, and nickel is frequently used for barrier layer. Nickel dissolves into the molten Sn-Ag-Cu alloy during the soldering process, and the ternary solder becomes a Sn-Ag-Cu-Ni quaternary melt. The phases formed at the Sn-Ag-Cu/Ni solder joints are mixing results of solidification and interfacial reactions. This study prepared the Sn-Ag-Cu-Ni alloys of various compositions. DTA was used to determine their cooling and heating curves. The solidified alloys were metallographically examined. No ternary or quaternary compounds were found. The knowledge of the primary solidification phases, phase formation sequences and the reaction temperatures determined in this study were put together with all the available liquidus projections of the constituent ternary systems to determine the liquidus projection of the Sn-rich quaternary Sn-Ag-Cu-Ni system. The knowledge was then used to interpret the solidification behaviors of the Sn-Ag-Cu-Ni alloys.

5:05 PM
Some Aspects of the Evolution of the Microstructure of Pb Free Solder Joints: *Eric J. Cotts*[1]; *Lawrence P. Lehman*[1]; [1]Binghamton University, Physics & Matls. Sci., Sci. Two, PO Box 6000, Binghamton, NY 13902-6000 USA

Changes in the metallurgy of solder joints has led to new challenges in understanding the evolution of their microstructure. The constituents (e.g. Cu, Ag) added to Sn to lower its melting point and increase its wettability as a Pb free solder, precipitate as intermetallics in the solder matrix, and may form compounds at interfaces as well. Thus the complexity of the problem of solder joint reliability has increased, and so has its importance, as these precipitates can significantly affect the mechanical properties of solder joints. The formation of intermetallic compounds at solder/metallization interfaces, and the evolution of precipitates in the solder matrix must be understood if reliable constitutive relations are to be developed for these materials. To this end we have examined precipitate formation and evolution in Pb free solder matrices and at solder/substrate interfaces for different reflow profiles on Ni or Cu metalizations. Support from the National Science Foundation, DM0218129 is gratefully acknowledged.

5:30 PM
Thermal Gradient in SnAg3.5 Solder Bumps Under Current Stressing: *S. H. Chiu*[1]; T. L. Shao[1]; Chih Chen[1]; D. J. Yao[2]; C. Y. Hsu[3]; [1]National Chiao Tung University, Dept. of Matl. Sci. & Engrg., 1001 Ta Hsueh Rd., Hsin-Chu 30050 Taiwan; [2]National Tsing Hua University, Inst. of Microelectromech. Sys., 101, Sect. 2 Kuang Fu Rd., Hsin-Chu 30050 Taiwan; [3]National Tsing Hua University, Dept. of Power Mechl. Engrg., 101, Sect. 2 Kuang Fu Rd., Hsin-Chu 30050 Taiwan

This study investigated of the thermal gradient and temperature increase in SnAg3.5 solder joints under electrical current stressing in flip-chip package by thermal infrared microscopy. The thermal gradients of both positive and negative tendencies were measured under different stressing conditions. The magnitude of the thermal gradient increases with the applied current. The measured thermal gradients reached 365°/C cm as powered by 0.59 A, yet there is no obvious thermal gradient was observed when the joints were powered less than 0.25 A. The temperature increase as a result of Joule heating was as high as 45.8°C when powered by 0.59 A, yet only 3.7°C when stressed by 0.19 A. Possible reasons that affect the thermal gradient and the temperature increase during current stressing are discussed.

Precipitation in Steels - Physical Metallurgy and Property Development: Precipitation in High Alloyed Steels

Sponsored by: AIST, AIST - Division V, AIST - Division VI
Program Organizers: Luis Ruiz-Aparicio, Duferco Farrell Corporation, Farrell, PA 16121 USA; Dengqi Bai, IPSCO Inc., Muscatine, IA 52761 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Tuesday PM — Room: La Galerie 3
September 28, 2004 — Location: Marriott New Orleans Hotel

Session Chair: Matthias Militzer, University of British Columbia, Vancouver, BC V6T 1Z4 Canada

2:00 PM
Coarsening of Secondary Hardening Carbides in a Hot-Work Tool Steel - Experiments and Simulation: *Harald Leitner*[1]; Helmut Clemens[1]; Michael Bischof[1]; Peter Staron[2]; Ernst Kozeschnik[3]; Franz Dieter Fischer[4]; Jiri Svoboda[5]; [1]Montanuniversität Leoben, Dept. Phys. Metall. & Matls. Testing, Franz-Josef-Strasse 18, Leoben 8700 Austria; [2]GKSS Research Center, Inst. for Matls. Rsch., Geesthacht 21502 Germany; [3]Graz University of Technology, Inst. for Matls. Sci., Welding & Forming, Graz 8010 Austria; [4]Montanuniversität Leoben, Inst. of Mech. & Erich Schmid Inst. for Matl. Sci., Franz-Josef-Strasse 18, Leoben 8700 Austria; [5]Academy of Sciences of the Czech Republic, Inst. of Physics of Matls., Brno 61662 Czech Republic

Hot-work tool steels are used for hot-forging dies, casting dies and extruding tools. Their use is based on an extraordinary combination of hot strength and remarkable toughness. Thermal fatigue and softening play the most important role with regard to tool life, and they are mainly influenced by coarsening of the nanometer-sized secondary hardening carbides. In the present work small-angle neutron scattering (SANS) was used to investigate microstructural changes during coarsening. SANS was employed to analyze the size distribution of precipitates in hot-work tool steel X 38 CrMoV 5-3 with different heat treatments. The investigations are compared with computer simulations based on a novel nonequilibrium thermodynamics model for describing the evolution of precipitates in multi-component, multi-particle, multi-phase systems. Both the experimental results and the simulations show that during overtempering complex changes in the population of secondary hardening carbides take place.

2:25 PM
Precipitation in Low Carbon 10% Nickel Steels: *Xian Jie Zhang*[1]; Earnest J. Czyryca[1]; [1]Naval Surface Warfare Center, Carderock Div., 9500 MacArthur Blvd., W. Bethesda, MD 20817 USA

Several secondary phases or micro-constituents, including nitride, carbide, austenite, and (M+A) constituent, precipitate at different stages of the metallurgical processing of low carbon 10% Ni high strength and ultra-high toughness steels. It is critical to differentiate their individual contributions to mechanical properties in the steel design and development process. A comprehensive study of several low carbon 10% nickel steels has been conducted to reveal processing-structure-property relations using a broad range of heat treatments, various mechanical tests, and advanced analytical techniques. It is concluded that metallurgical features other than precipitation strengthening are also important contributors to its superior combination of high strength and ultra-high toughness. These include low volume fraction and well-controlled morphology of inclusions, thermally stable fine martensite laths, and fine retained austenite islands.

2:50 PM
On the Precipitation Behaviour of a Ni and Al Alloyed Martensitic Tool Steel: *Stefan Erlach*[1]; Harald Leitner[2]; Michael Bischof[2]; Helmut Clemens[2]; Frederic Danoix[3]; Deni Lemarchand[3]; [1]Materials Center Leoben, Franz Josefstraße 13, Leoben Austria; [2]University of Leoben, Dept. for Physl. Metall. & Matls. Testing, Leoben Austria; [3]Universite de Rouen, Groupe de Physique des Materiaux, UMR CNRS 6634, Saint Etienne du Rouvray France

The combined precipitation of secondary hardening carbides and intermetallic phases is a well known effect to improve the mechanical properties of steels. For the controlled precipitation of nm-sized particles, the precipitation reactions which occur during aging must be known in order to define proper heat treatment parameters. The precipitation behaviour of a 0.4 C/2.5 Al/5.0 Ni wt% martensitic model alloy has been studied during isothermal aging at 610°C. The combination of high resolution methods like transmission electron microscopy, field ion microscopy and three-dimensional atom probe were applied to characterize the precipitation type, precipitation sequence and spatial distribution of the alloying elements. The precipitates were identified as different types of secondary hardening carbides and an intermetallic NiAl-based phase. The dependence of precipitation size on aging time, their nucleation sites as well as the evolution of the chemical composition will be reported.

3:15 PM Break

3:25 PM
EFTEM Investigations on Precipitates in Creep Resistant 9-12% Cr Steels: *Bernhard Sonderegger*[1]; Gerald Kothleitner[2]; Werner Rechberger[2]; Horst Cerjak[1]; [1]Graz University of Technology, Inst. for Matls. Sci. Welding & Forming, Kopernikusgasse 24, Graz, Austria A- 8010 Austria; [2]Graz University of Technology, Rsch. Inst. for Electron Microscopy & Fine Struct. Rsch., Steyrergasse 17, Graz, Austria A- 8010 Austria

9-12% chromium steels are well established materials for high temperature components in ultra efficient power plants. An important parameter for the creep resistance of these steels is the formation and interaction of different precipitate populations like MX, M23C6, Laves phase and Z-phase. In this work, TEM/ EFTEM studies were carried out on samples of the European COST steel CB8, which had been creep loaded at 923K for up to 16000 h. Enhanced evaluation methods are applied to determine the size, volume fraction and frequency of the precipitates in samples of varying thickness and arbitrary precipitate size distributions. The results clearly show growth and coarsening of the precipitates in the course of in-service exposure.

3:50 PM
Effect of Precipitation on Creep Properties of Certain Cast H-Series Austenitic Stainless Steels: *Govindarajan Muralidharan*[1]; Philip J. Maziasz[1]; Neal D. Evans[1]; Michael L. Santella[1]; Ken C. Liu[1]; James G. Hemrick[1]; Vinod K. Sikka[1]; Roman I. Pankiw[2]; [1]Oak Ridge National Laboratory, Metals & Ceram. Div., Bldg. 4508, MS-6083, 1 Bethel Valley Rd., Oak Ridge, TN 37831-6083 USA; [2]Duraloy Technologies, Inc., Engrg. & Quality, 120 Bridge St., Scottdale, PA 15683-1748 USA

Cast H-Series austenitic steels (HK, HP, and micro-alloyed HP) are used extensively for a broad range of high-temperature applications. The H-Series stainless steels have evolved over many years of complex alloy development that resulted in the addition of various alloying elements by trial-and-error methods. It is understood that further improvements will be possible only through a detailed understanding of the composition-microstructure-property relationships. The native microstructure established in these fully-austenitic alloys consists of an austenite matrix with finer dispersions of carbides (Cr-rich $M_{23}C_6$ or Nb-rich MC, depending on the alloy) in the matrix along with clusters of NbC in the interdendritic regions and dispersions of $M_{23}C_6$ along the seams between colonies of dendrites. Using a combination of thermodynamic modeling, microstructural characterization, and mechanical property measurements, we have obtained some understanding of the relationship between the precipitation and creep properties of these alloys and will be highlighted in the talk.

4:15 PM
Control of Grain Size in Nb Alloyed Creep Resistant Steels: *Chia Yuin Wong*[1]; George Fourlaris[1]; [1]University of Wales, Matls. Rsch. Ctr., Singleton Park, Swansea SA2 8PP UK

Coarsening of second phase particles in a metallic matrix plays an important role in many metallurgical phenomena, such as the tempering of martensite, grain growth, precipitation hardening and creep deformation. The broad definition of the particle coarsening reaction relates to the growth of second phase particles without significant change in the matrix solute content. The main thrust of this experimental work is to establish the particle coarsening rates of one or more species of precipitate in a range of Nb alloyed creep resistant stainless steels. Moreover, a mathematical model will be formulated to predict grain growth inhibition as well as to facilitate the control of microstructure by thermal treatment and the attendant control of mechanical properties.

Primary Operations and Product Quality: Session I

Sponsored by: AIST, AIST - Division VI
Program Organizers: Mark R. Blankenau, SeverStal NA, Dearborn, MI 48121 USA; Amy Bailey, TXI - Chaparral Steel, Midlothian, TX 76065 USA; John G. Speer, Colorado School of Mines, Metallurgical and Materials Engineering, Golden, CO 80401 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Tuesday PM	Room: La Galerie 1
September 28, 2004	Location: Marriott New Orleans Hotel

Session Chairs: Mark R. Blankenau, SeverStal NA, Dearborn, MI 48121 USA; Timothy L. Mitchell, NorthStar BlueScope Steel LLC, Quality Assurance, Delta, OH 43522 USA

2:00 PM
Hot Ductility Improvement in the Peritectic Steel containing Vanadium by Application of High Temperature Deformation: *Ahmad Rezaeian*[1]; F. Zarandi[1]; D. Q. Bai[2]; S. Yue[1]; [1]McGill University, Metals & Mining & Metall. Engrg. Dept., 3610 Univ. St., Wong Bldg., Montreal, Quebec H3A 2B2 Canada; [2]IPSCO Inc., R&D, Armour Rd., PO Box 1670, Regina, SK S4P 3C7 Canada

On solidification, peritectic steels develop coarse as-cast grain sizes and large columnar grains that enhance grain boundary separation as the grain boundary crack aspect ratio is increased. Furthermore, microalloying additions such as V and Nb can encourage intergranular precipitation. Both these effects can result in loss of hot ductility and cracking during the unbending stage of continuous casting. Tensile specimens were melted and solidified in situ and the effect of pre-deformation applied in the very high temperature region of single phase austenite was studied. According to the current results, it seems that a deformation in the very high temperature region of austenite (below the solidus) improves the hot ductility at the unbending stage. The beneficial effect of such deformation on the hot ductility varies with the unbending temperature. In addition, the effect of very high temperature deformation on the hot ductility was compared in reheated and in situ melted specimens. The aforementioned issues will be discussed in this paper.

2:25 PM
A Defect FMEA Approach to Determining Root Cause of Complex Iron Oxide Based Laminations in Sheet Steel: *Bill Barker*[1]; Dennis Hreso[2]; [1]Procoil Company; [2]USS

Development of a complex FMEA by cross functional team of steelmaking and Hot Rolling Operators, quality assurance metallurgists and research scientists served as the basis of focused hot mill process improvements to reduce the occurrence and severity of Iron Oxide based surface and subsurface laminations. Part of the process used in assessing ratings for occurrence and severity included qualitative SEM analysis of defect samples collected throughout the finishing operations. This paper will review the process of developing the Defect FMEA, integration of the SEM work to assist in developing the assessments, and the focus of the process improvements implemented.

2:50 PM
The Effect of Austenite Grain Size on Hot-Ductility of Steels: *Suk-Chun Moon*[1]; Rian Dippenaar[1]; [1]University of Wollongong, Steel Inst., Northfields Ave., Wollongong, NSW 2522 Australia

Excessive grain growth, especially at the roots of oscillation marks, has been implicated as a possible cause of reduced ductility during unbending of continuously cast slabs. In an attempt to isolate the effect of grain size from the influence of alloying elements, three plain carbon steels were used to determine the relationship between hot-ductility and grain size. High-temperature tensile tests of re-heated as well as in-situ cast specimens in the temperature range 1100°C to 700°C were done on a Gleeble 3500 thermo-mechanical processor. The detrimental effect of grain size was most severe in alloys of near peritectic composition and moreover, in specimens directly cast, austenite grains were of columnar nature as opposed to equi-axed structures in the other alloys. The presence of large austenite grains seemed to be more detrimental to hot-ductility in the austenitic region than an as-cast structure, at least under the pertaining experimental condition.

3:15 PM
Improvement of Surface Quality on Type 304 and 316 Stainless Steel Bloom by Continuous Casting: *Young Mo Kim*[1]; Young Jin Jung[3]; Dai Ryoung Kim[2]; [1]RIST, Iron & Steel Process Div., Hyoja-dong san 32, Nam-

gu, Pohang, Kyoungbook 791-330 Korea; [2]Kyoungbook National University, Metallurgl. Engrg. Dept., Sangyuk-dong 1370, Buk-gu, Daegu 702-701 Korea; [3]POSCO, Steel Plate Rsch. Lab., Dongchon-dong 1, Namgu, Pohang, Kyoungbook 790-785 Korea

In this study, in order to improve the surface quality of blooms in continuous casting process for the production of stainless blooms, the effects of chemical composition, viscosity and basicity of mold powder on the prevention of surface defects were investigated. The main results obtained are as follows: 1) In plant application tests of new mold powder for the production of stainless blooms, satisfactory results were obtained. The optimum composition of the mold powder was determined and the quality of the surface was improved by the application. 2) It is possible to reduce the number of surface grinding needed for the removal of surface defects by the application. 3) The main cause of the surface defects was found to be the penetration of carbon contained in mold powder. Chromium carbide can be formed by the carbon penetration and can cause surface cracks along to the grain boundaries.

3:40 PM Break

4:10 PM
Transient Casting Practices and their Effects on Steel Cleanness at CSP Port Talbot Works UK: *Paul Thomas*[1]; Alun H. Thomas[2]; Mike Jefford[3]; [1]University of Wales, Engrg. Doctorate Ctr., Matls. Rsch. Ctr., Sch. of Engrg., Singleton Park, Swansea SA2 8PP UK; [2]Corus Strip Products, Port Talbot UK; [3]Corus Strip Products, Port Talbot UK

For critical applications such as thin-wall tinplate products, only steel cast during 'steady-state' conditions is selected. Slab cast over defined lengths before and after a ladle change is down-graded to less demanding applications, irrespective of cleanness. This plant-based study evaluated steel cleanness during continuous casting, ladle change practices, with the steel reservoir in the tundish at different levels. It showed marked variations in size and morphology of the non-metallic inclusions, as well as in the oxygen content of the steel slab over a ladle change period.

4:35 PM
Inside Morphology of Large Inclusions in Steel: Liping Wang[1]; *Lifeng Zhang*[2]; Kai Qian[1]; [1]Shougang Research Institute of Technology, Shougang Grp., Shougang, Shijingshan Dist., Beijing 100041 China; [2]University of Illinois, Mechl. & Indust. Engrg., 345 Mech. Engrg. Bldg., 1206 W. Green St., Urbana, IL 61801 USA

Large inclusions are extracted from Si-Mn steel and Si-Al-Ba steel by Slimes test. The extracted inclusions are then sectioned by polishing after sticked on the surface of a glass slice. Inside morphology of inclusions are therefore revealed. The results indicate that the outside morphology and composition of some inclusions are totally different from inside. There are many spherical clusters and dendrites in the core of inclusions, though these inclusions are apparently spherical with very thin shell (1-5μm) at outside. The reason of this inside morphology is theoretically discussed. This inside morphology cannot be clearly shown by traditional microscope observation of polished steel samples.

5:00 PM
Inclusion Control in Tire Cord Steels: *Lifeng Zhang*[1]; Yong Wang[2]; Deguang Zhou[2]; Xiongguang Hu[2]; Kai Qian[2]; [1]University of Illinois, Mechl. & Indust. Engrg., 345 Mech. Engrg. Bldg., 1206 W. Green St., Urbana, IL 61801 USA; [2]Shougang Research Institute of Technology, Shougang Grp., Shougang, Shijingshan Dist., Beijing 100041 China

The current production process of tire cord steels is reviewed. Inclusion and segregation requirements for the tire cord steel are discussed. The technologies to control inclusions in tire cord steels are reviewed including steel deoxidizer choice, steel refining, ladle slag treatment, calcium treatment, tundish operations, electromagnetic stirring, and soft reduction during continuous casting. Control of the total oxygen, nitrogen, phosphorus, sulfur in tire steel is also discussed. The production practice of tire cord steel at Shougang Steel Group is summarized.

5:25 PM
Development of Magnesia-Carbon Zonal Lining in 150T LF-CC Ladle to Achieve Highest Lining Life in SAIL Plants: *Swapan Kumar Garai*[1]; Purimetla Chintaiah[1]; Nirmal Kanti Ghosh[1]; Pulak Barua[1]; Devi Prasad Chakraborti[1]; [1]RDCIS, PO Doranda, Ranchi, Jharkhand 834002 India

Steel malting shop No. 2 of Rourkela Steel Plant, Steel Authority of India Limited, India is equipped with 2 Nos. of BOF and 17 Nos. of steel ladles of capacity 150T each for production of 1.5 MT steel through BOF-LF-CC route. An average steel ladle lining life of 46 heats was obtained in 2003 - 04 using high alumina bricks in bottom, metal zone and MgO-C bricks in slag zone of the ladle as working lining. Ladle wear profile of few campaigns were studied and based on wear profile a zonal lining design was developed using different quality magnesia-carbon bricks for working lining of ladles. Thermal regime in the lining was modified incorporating ceramic fibre based insulation on shell and basic granules as back fill mass in between working and safety lining to maintain same shell temperature as in the case of normal ladles. Initially two trials were conducted which gave life of 100 heats and 80 heats which is highest among four integrated SAIL plants. Further 10 trials were done with in-house developed MgO-C bricks which gave average life of 81 heats with maximum 88 heats. Action has been initiated for implementation of full MgO-C ladle lining in all ladles.

Rhenium and Rhenium Containing Alloys: Rhenium

Sponsored by: TMS - Structural Materials Division, SMD-Refractory Metals Committee
Program Organizer: Todd A. Leonhardt, Rhenium Alloys, Research and Development, Elyria, OH 44036-0245 USA

Tuesday PM Room: Grand Ballroom J
September 28, 2004 Location: Marriott New Orleans Hotel

Session Chairs: Gary A. Rozak, H.C. Starck, Fabricated Products, Cleveland, OH 44117 USA; Bill W. Buckman Jr., Refractory Metals Technology, Pittsburgh, PA 15236-6055 USA

2:00 PM
Processing of Rhenium by Chemical Vapor Deposition: *Gautham Ramachandran*[1]; Art J. Fortini[1]; [1]Ultramet, 12173 Montague St., Pacoima, CA 91331 USA

Chemical Vapor Deposition (CVD) is a viable and efficient technique for the fabrication of rhenium components. The primary advantages of CVD are its ability to fabricate net or near net shapes, be applied towards a broad range of materials, maintain high levels of purity, deposit materials near theoretical density, and fabricate coatings or free-standing structures. A general background of CVD processing will be presented followed by a more detailed analysis of the issues related to processing of rhenium components.

2:30 PM
The Effects of Rolling Mode on the Mechanical Strength and Crystallographic Texture of Rhenium Metal: *Omar S. Es-said*[1]; Todd A. Leonhardt[2]; [1]Loyola Marymount University, One LMU Dr., Los Angeles, CA 90045 USA; [2]Rhenium Alloys Inc., 1329 Taylor St, Elyria, OH 44035 USA

This project investigated the effect of varying the rolling direction on the strain hardening of rhenium sheet in an effort to increase the tensile strength. The 0, 45, and 90° rolling direction were experimented with a 10% reduction between annealed cycles. The annealing times varied from 30 minutes for the first four anneals, to 20, 15, and 10 minutes for the subsequent annealing intervals. A total reduction 74.5% was achieved with a density of 99.9%. As will be discussed the 45° rolling direction gives the highest hardness values which relates to orientation and texture of the hexagonal closed packed crystal.

3:00 PM
CVD Rhenium - Mechanical Properties and Microstructural Evolution: *Gautham Ramachandran*[1]; [1]Ultramet, 12173 Montague St., Pacoima, CA 91331 USA

The currently available database of rhenium mechanical properties is limited and a fundamental understanding of crystallography and microstructural evolution in rhenium is lacking. The goal of this ongoing research is to develop a better understanding of processing-structure-property relationships in CVD rhenium. A matrix of tests is underway to assess the mechanical properties of CVD rhenium and compare it with rhenium manufactured via other processing methods. Also, structure and crystallography of CVD rhenium are being investigated in an attempt to understand microstructural evolution and grain boundary migration. Results thus far indicate significant differences in rhenium mechanical properties as a function of processing and microstructure. These results will be presented along with the findings of a microstructural evolution analysis as a function of processing, deformation, and post-process heat treatments.

3:30 PM
The Constitutive Behavior of Rhenium: Shuh-Rong Chen[1]; John Bingert[1]; Laura Beth Addessio[1]; Benjamin Lyman Henrie[1]; *Ellen Cerreta*[1]; George T. Gray[1]; [1]Los Alamos National Laboratory, MST-8, MS G755, Los Alamos, NM 87545 USA

The effect of texture, temperature, and strain-rate on the mechanical behavior of cold rolled, powder metallurgy rhenium has been examined. The material displays characteristic high rates of work hardening upon compressive loading. The yield stress and work hardening behavior in compression are sensitive to strain rate and temperature and to a greater extent texture. The microstructure and substructure have been examined as a function of strain and are correlated with the observed stress-strain response. The Mechanical Threshold Strength (MTS) model has been used to capture the mechanical response for this plate of rhenium. Parameters for the constitutive relations for cold rolled rhenium were derived for the MTS model. The model is in good agreement with the observed experimental data and therefore substantiates the use of MTS for describing the high strain rate deformation behavior of rhenium.

4:00 PM Break

4:10 PM
Plastic Deformation and Fracture Behaviors of Diffusion Bonded Stocks of Cold-Rolled Rhenium Plates: *Xian J. Zhang*[1]; Amy C. Stauffer[1]; [1]Naval Surface Warfare Center, Carderock Div., 9500 MacArthur Blvd., W. Bethesda, MD 20817 USA

The complexities of manufacturing processes of diffusion bonded stocks of cold-rolled HIP (hot isostatically pressed) rhenium plates result in several microstructural features affecting its mechanical properties, including porosity, grain size, grain orientation, texture, and bonding strength. A comprehensive metallographic and fractographic study of a number of bonded stock tensile samples tested over a temperature range of 70°F to 3700°F was conducted to reveal key factors controlling their plastic deformation and fracture behavior. It is concluded that: 1) twining is the dominating plastic deformation mechanism, 2) intergranular fracture is the main fracturing mode, 3) inherent excellent ductility of individual rhenium grains is limited by mis-orientations among neighboring grains and bonding strength of plates, 4) bonding strength appears to be the determining factor for the ductility of bonded stock tensile sample, and 5) porosity of the examined samples, formed in the HIP process, does not play a significant role.

4:40 PM
Making and Shaping of Rhenium: *Todd A. Leonhardt*[1]; Sean R. Agnew[2]; [1]Rhenium Alloys, Inc., 1329 Taylor St., Elyria, OH 44036 USA; [2]University of Virginia, 116 Engineer's Way, Charlottesville, VA USA

The effect of cold rolling on the structure and tensile behavior of rhenium was extensively researched by Rhenium Alloys Inc. An objective of the research was to determine, if cross rolling imparts a better microstructure or mechanical properties to pure rhenium plate products in comparison with simple longitudinal rolling direction. Metallography, hardness and x-ray texture measurements were performed to examine the grain size, orientation, hardness and morphology between the two rolling processes. X-ray texture measurements of the as-sintered material compared to both the long-rolled and cross-rolled of the hexagonal close packed crystals were investigated. Finally, room and elevated temperature tensile testing were performed along the rolling and transverse directions of both types of process to investigate isotropic and anisotropic behavior of cold rolled rhenium.

The Accelerated Implementation of Materials & Processes: Microstructure Modeling: 1st Principle Theory, Phase Field & Thermodynamic Modeling

Sponsored by: TMS - Structural Materials Division, TMS - ASM/MSCTS-Thermodynamics & Phase Equilibria Committee, TMS - EMPMD/SMD-Chemistry & Physics of Materials Committee, TMS - MPMD-Computational Materials Science & Engineering-(Jt. ASM-MSCTS)
Program Organizers: Rollie E. Dutton, Air Force Research Laboratory, AFRL/MLLMP, WPAFB, OH 45433 USA; John E. Allison, Ford Motor Company, Materials Science and Advanced Engineering, Dearborn, MI 48124-2053 USA; John J. Schirra, Pratt & Whitney, East Hartford, CT 06108 USA; Axel van de Walle, Northwestern University, Materials Science and Engineering, Evanston, IL 60208-3108 USA

Tuesday PM — Room: Mardi Gras Ballroom H
September 28, 2004 — Location: Marriott New Orleans Hotel

Session Chair: John E. Allison, Ford Motor Company, Matls. Sci. & Advd. Engrg., Dearborn, MI 48124-2053 USA

2:00 PM
Effect of Incoherent Oxide Particles on Grain Boundary Motion - A Phasefield Approach: *Sundar Amancherla*[1]; Yunzhi Wang[2]; Ramkumar Oruganti[1]; P. R. Subramanian[3]; Dheepa Srinivasan[1]; [1]GE India Technology Center, Matls. Rsch. Lab., EPIP, Phase-2, Whitefield Rd., Bangalore, Karnataka 560066 India; [2]Ohio State University, Dept. of Matls. Sci. & Engrg., 477 Watts Hall, 2041 College Rd., Columbus, OH 43210 USA; [3]GE Global Research, Ceram. & Metallurgl. Tech., PO Box 8, K1-MB265, Schenectady, NY 12301 USA

It is well-known that grain refinement in structural materials can result in improved mechanical properties. Recent research has been concentrated on producing fine-grain-sized materials with sub-micron to nanometer grain sizes. Fine-grained-structures tend to coarsen high temperatures. However, a distribution of second-phase particles such as oxides could inhibit grain coarsening. To be able to tailor the fine-grain structure for high temperature applications, an understanding of the grain boundary motion becomes significant. Modeling the effect of oxide particles on the grain boundary motion can accelerate the understanding and the design of thermally stable fine-grain-sized materials. This paper focuses on the phase-field modeling technique for understanding grain boundary motion in the presence of incoherent second-phase particles with little or no solubility in the matrix. The construction of the model and the application of the model to design a thermally stable structure with optimum distribution of the second-phase particles will be discussed in detail.

2:25 PM
Dissolution Kinetics Study of Eutectic Al2Cu Phase in a Cast 319 Aluminum Alloy: *Mei Li*[1]; Jacob Zindel[1]; Larry Godlewski[1]; William Donlon[1]; John E. Allison[1]; [1]Ford Motor Company, Matls. Sci. & Advd. Engrg., 2101 Village Rd., Dearborn, MI 48124 USA

In recent years there has been an increasing need for robust simulation methods and tools to accelerate the optimization of process and product design of cast components. At Ford, the goal of cast aluminum research is to provide tools that simulate casting solidification and heat treatment and predict microstructure, mechanical properties and durability in a cast component. The vision is to create and test "Virtual Aluminum Castings", reducing the need for physical prototypes. This talk describes the development of a dissolution kinetic model for quantifying the influence of heat treatment and its application to study the dissolution kinetics of eutectic Al2Cu phase in a cast 319 aluminum alloy. The multicompenent thermodynamic and kinetic behavior of the system is taken into account using the DICTRA software and the influence of alloying elements coring generated during solidification is discussed. The predictions of the model are found to be in good agreement with experimental results.

2:50 PM
First-Principles-Aided Identification of Electron-Hole Traps in X-Ray Detector Scintillators: *Axel van de Walle*[1]; Sundar Amancherla[2]; Mark D. Asta[1]; Steven J. Duclos[2]; [1]Northwestern University, Matls. Sci. & Engrg., 2225 N. Campus Dr., Evanston, IL 60208-3108 USA; [2]GE India Technology Center, Matls. Rsch. Lab., EPIP, Phase-II, Whitefield Rd., Bangalore 560066 India; [2]GE India Technology Center, Matls. Rsch. Lab., EPIP, Phase-II, Whitefield Rd., Bangalore 560066 India

X-ray detectors often rely on scintillation materials, in which high-energy X-ray photons create electron-hole pairs that subsequently recombine, resulting in the emission of a larger number of lower-energy photons. While an ideal scintillator should only emit light while the material is exposed to X-rays, a typical detector exhibits an unwanted "afterglow" due to the trapping of excited electrons or holes in defect levels, followed by their slow, thermally activated, release. In order to reduce this unwanted phenomenon, it is important to identify the defects responsible for the afterglow. Experimental techniques such as thermoluminescence are valuable in determining the energetics of such defects, however they provide little information about their physical structure. We illustrate how first-principles calculations can provide helpful guidance to accelerate the process of identifying the defects responsible for afterglow. Our investigation focuses on Europium-doped Yttria scintillators and employs density functional theory (DFT) calculations to identify the points defects most likely to introduce defect levels in the gap associated with an afterglow. The limitations of DFT in the context of the determination of excited states energy levels are discussed, and practical way to alleviate them are presented.

3:15 PM Break

3:30 PM Invited
PrecipiCalc Simulations for the Prediction of Microstructure/Property Variation in Aeroturbine Disks: *Greg B. Olson*[1]; Herng-Jeng Jou[2]; [1]Northwestern University, Dept. Matl. Sci. & Engrg., 2225 N. Campus Dr., Evanston, IL 60208 USA; [2]QuesTek Innovations LLC, 1820 Ridge Ave., Evanston, IL 60201 USA

In support of a new methodology of accelerated development and qualification of new materials, the PrecipiCalc(TM) software has been developed as an efficient, high-fidelity 3D multiphase precipitation simulator grounded in computational thermodynamics and multicomponent diffusional nucleation and growth models incorporating interfacial dissipations. With extensive validation under a major experimental program, the software has been successfully applied to the accurate and rapid simulation of multiscale (from nano to micrometer), multimodal gamma-prime microstructure development in IN100 Ni-based aeroturbine disk alloys under complex commercial heat-treatment processing. Integration of PrecipiCalc with FEM heat transfer simulation and a strength model has demonstrated accurate prediction of property variation for accelerated process optimization and probabilistic modeling of design minimum properties.

3:55 PM
Phase-Field Engineering Model for Heat Treatment Applications in Ni-Base: *You-Hai Wen*[1]; Fan Zhang[2]; Sarath Menon[1]; Billie Wang[3]; Yunzhi Wang[3]; Jeff Simmons[4]; [1]UES Inc., 4401 Dayton-Xenia Rd., Dayton 45432 USA; [2]CompuTherm LLC, 437 S. Yellowstone Dr., Madison, WI 53719 USA; [3]Ohio State University, Dept. Matls. Sci. Engrg., 2041 College Rd., Columbus OH 43210 USA; [4]Air Force Research Laboratory/MLLM, Wright-Patterson AFB, OH USA

This presentation summarizes our effort towards developing a phase-field engineering model for modeling two-phase microstructure (gamma and gamma prime) in Ni-base alloys during heat treatment. Ni-base commercial alloys typically contain more than a dozen of components and the two-phase microstructure evolution is controlled by the diffusion of these components. Linking phase-field with a full multi-component treatment of the thermodynamics is a difficult one, due to the complexity of commercial alloy systems, and is an active area of research by a number of research groups. As an alternative, we propose a simplified pseudo-binary model to treat multi-component Ni-based alloys in which effective mobility and rescaled free energy are introduced to reflect the collective behavior of the alloy under investigation. The idea is tested in a 5-component alloy that closely mimics the precipitation behavior of the Rene88DT. Comparison between simulation and experimental results will be presented. Work completed under Air Force Contract # F33615-01-C-5214.

The Effects of Microstructure and Property Homogeneity/Variability on Product Performance: Session I

Sponsored by: AIST, AIST - Division VI
Program Organizers: J. M. Rodriguez-Ibabe, CEIT Spain; Roger Pradhan, ISG Reseach; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Tuesday PM — Room: Grand Ballroom M
September 28, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Roger Pradhan, ISG Labs, Bethlehem, PA 18015 USA; John G. Speer, Colorado School Mines, Golden, CO 80401 USA

2:00 PM
Texture Gradient of As-Cast Low-Carbon Thin Steel Slab: *Pingguang Xu*[1]; Fuxing Yin[1]; Kotobu Nagai[1]; [1]National Institute for Materials Science, Steel Rsch. Ctr., 1-2-1, Sengen, Tsukuba, Ibaraki 305-0047 Japan

The compact strip production technology composed of thin slab casting and directly hot rolling has attracted abroad attention due to its apparent cost advantage. In this presentation, the microstructural and textural variations in the through-thickness direction and their effects on the plastic anisotropy gradient in a copper-containing thin-slab-cast low-carbon steel were investigated. The textures in all through-thickness layers are composed of mainly {111}<uvw> and relatively weak {001}{uvw} components, while the former component reaches its maximum texture intensity in the layer near S=0.4 (S is the normalized distance from the slab center to the specific layer, to the slab surface is 1.0). Though the weakest {111}<uvw>-fiber intensity occurs in the surface layer, it still leads to better plastic anisotropy and the relatively stronger {111}<uvw>-fiber intensity occurring in the center layer results in the lowest r_m value, showing that the composition segregation and inclusion particles have an apparently detrimental influence on the plastic anisotropy.

2:30 PM
High Strength Low Alloy (HSLA) Steels for Automotive Applications: *Sarah-Jane Bell*[1]; G. Fourlaris[1]; [1]University of Wales, Matls. Rsch. Ctr., Sch. of Engrg., Swansea SA2 8PP UK

This study assesses the effect of variable annealing sequences on the microstructural evolution and attained mechanical properties of two experimental HSLA steels, based on combined titanium-vanadium additions and titanium only additions and compares them to a commercial (niobium only) HSLA grade. Moreover, for each HSLA grade, the optimum annealing temperature is established, which results in improved mechanical property characteristics. Since micro-alloying elements influence the grain size differently, a different grade may produce the required strength at lower annealing temperatures. It was found that the Nb grade had the finest grain size and exhibited the higher strength at an optimum annealing temperature of 670°C.

3:00 PM
Subcritical Heat Treatment of Cold Rolled Multi-Phase TRIP Steel: *Taeki Jeong*[1]; Elhachmi Es-sadiqi[2]; Stephen Yue[1]; [1]McGill University, Dept. of Metals & Matls. Engrg., 3610 Univ. St., Montreal, Quebec H2X 3R2 Canada; [2]Natural Resources Canada, Matls. Tech. Lab. - CANMET, 568 Booth St., Ottawa, Ontario K1A 0G1 Canada

TRIP (TRansformation Induced Plasticity) steels can be used in the cold rolled and "TRIP annealed" condition. TRIP annealing is designed to produce the complex microstructures, comprised of ferrite, bainite, retained austenite, which achieve the best combination of strength and formability. Thus, the processing of these steels requires careful selection and delicate control of temperatures and holding times. In this context, this project has been carried out to design an alternative process for TRIP steel, using a relatively simple subcritical heat-treating process. Basically, the concept is to cold roll the TRIP steel to produce strain induced martensite, as well as work hardened ferrite and bainite, and then to "conventionally" anneal the steel to produce tempered martensite and bainite, as well as recrystallized ferrite. The microstructural evolution during this subcritical heat treatment, and the subsequent mechanical properties will be presented in this paper.

3:30 PM Break

4:00 PM
Influence of Grain Refinement on the Mechanical Properties of a Dual Phase Steel: *Prodromos Tsipouridis*[1]; Ewald Werner[1]; Christian Krempaszky[1]; Ernst Tragl[2]; Andreas Pichler[2]; [1]Christian Doppler Laboratorium für Moderne Mehrphasenstähle/Technische Universität München, Lehrstuhl für Werkstoffkunde und Werkstoffmechanik, Boltzmannstraße 15, Garching b. München, 85747 Germany; [2]voestalpine stahl Linz, B3E R&D, VOEST-ALPINE Straße 3, Postfach 3, Linz A-4031 Austria

The influence of severe plastic deformation (by means of conventional cold-rolling) on the microstructure of a pre-processed dual-phase steel was studied with respect to grain refinement and its impact on the mechanical properties of the steel. The deformed material is finally annealed by applying appropriate heat treatments, including intercritical annealing and HDG cycles, according to the starting microstructure and the deformation degree. Microstructure investigations via light and electron microscopy show that ultrafine grain formation is achievable, reaching a ferrite mean grain size of ~1.5μm. Martensite grains are even finer. Tensile tests confirm the superior performance of such fine-grained microstructures, compared with the starting material. The ultimate tensile strength and the total elongation exhibit high values, while the yield stress remains at a remarkably low level (below 400MPa). Finally the mechanical properties can be correlated with the microstructural features of the material (grain size, volume fraction and geometrical arrangement of martensite).

4:30 PM
Recrystallisation and Grain Size Control in Novel Interstitial Free (IF) Strip Steels: *Shgh Woei Ooi*[1]; G. Fourlaris[1]; [1]University of Wales, Sch. of Engrg., Singleton Park, Swansea SA2 8PP UK

One of the key factors affecting the attendant strength and formability characteristics of Interstitial Free (IF) steels is the control of recrystallisation temperature, as well as, the grain size of annealed cold rolled strips. Two novel IF steel grades were investigated, one based on combined vanadium and titanium additions and the other based on titanium only additions. It is identified that novel Ti-V IF strips steel may have a potential for achieving very high formability values employing lower dwell temperatures during annealing. The crucial role of Ti(CN) in retarding the recrystallisation behaviour in IF strip steel has been confirmed. Moreover, it has also been confirmed the key role of carbide precipitation, within ferrite, in controlling the obtained fine recrystallised ferrite grain size in Ti-V IF strips steels.

Titanium for Healthcare, Biomedical, and Dental Applications: Processing

Sponsored by: TMS - Structural Materials Division, Japan Institute of Metals, TMS - SMD-Titanium Committee, TMS - SMD-Corrosion and Environmental Effects Committee-(Jt. ASM-MSCTS)

Program Organizers: Carl Boehlert, Alfred University, School of Ceramic Engineering and Materials Science, Alfred, NY 14802 USA; Dhanesh Chandra, University of Nevada, Metallurgical and Materials Engineering, Reno, NV 89557 USA; Masahiko Ikeda, Kansai University, Department of Materials Science and Engineering, Suita, Osaka 564-8680 Japan; Mitsuo Niinomi, Toyohashi University of Technology, Department of Production Systems Engineering, Toyohashi 441-8580 Japan

Tuesday PM	Room: Mardi Gras Ballroom D
September 28, 2004	Location: Marriott New Orleans Hotel

Session Chair: Masahiko Ikeda, Kansai University, Dept. of Matls. Sci. & Engrg., Suita, Osaka 564-8680 Japan

TUESDAY PM

2:00 PM Invited
Surface Bioactivity of Ti Implants: *Otto Wilson*[1]; M. Ashraf Imam[2]; [1]Catholic University, Dept. of Biomed. Engrg., BONE/CRAB Lab., Washington, DC USA; [2]Naval Research Laboratory, Washington, DC USA

Controlled surface treatments of Ti bioimplants have revolutionized the field of bone reconstruction and hard tissue engineering. This result stems from the high degree of integration between Ti and bone that can be achieved when the surface chemistry and microstructure of the Ti implant are optimized. The most beneficial surface treatments to date include controlled oxidation to convert Ti to titania, incorporation of calcium and phosphate, and the introduction of porosity. An overview of the surface modification of Ti bioimplants for enhanced bioactivity will be presented with a focus on Ti surface modification methodologies and their impact on bone growth at the whole tissue, cellular, and subcellular levels.

2:25 PM
A Clean Binder System for Powder Injection Molding Titanium Parts: *Eric A. Nyberg*[1]; Kevin L. Simmons[1]; K. Scott Weil[1]; [1]Pacific Northwest National Laboratory, Matls. Dept., 902 Battelle Blvd., PO Box 999, Richland, WA 99352 USA

The use of titanium in medical implants continues to expand as its advantages in dramatically reducing the overall time of recovery and rehabilitation and in improving patient comfort become more apparent. However, more rapid progress will be made as the cost of titanium processing is reduced. One manufacturing technique that is promising in this regard, but remains fraught with technical challenges is powder injection molding (PIM). PIM is an economical, net-shape process for manufacturing large volumes of complex-shaped parts. However this process has found only limited use in the manufacture of titanium, namely because of the metal's extreme reactivity with oxygen, nitrogen, and carbon particularly at elevated temperature, i.e. during binder burn-out and sintering. These impurities dramatically degrade the mechanical properties of titanium and its alloys. Traditional methods of PIM employ a high volume fraction of polymer in the metal powder/binder mixture, which in addition to being difficult to remove entirely during burn-out, has a tendency to degas in the removal process and cause undesired dimensional and shape changes in the component. We have recently developed a binder system that is unique because only a small volume fraction of binder (~5 - 10 vol%) is required for injection molding; the remainder of the mixture consists of the alloy powder and binder solvent. Because of the nature of decomposition in the binder system and the small amount used, the binder is eliminated almost completely from the pre-sintered component during the initial stage of a two-step heat treatment process. Results from impurity testing have shown that the final densified titanium product contains the same level of carbon as the original starting powder.

2:50 PM
Effect of Severe Plastic Deformation Process Using ECAP on Microstructure and Mechanical Properties of Beta-Type Titanium Alloys for Biomedical Applications: *Guna Warman*[1]; Mitsuo Niinomi[1]; Toshikazu Akahori[1]; [1]Toyohashi University of Technology, Production Sys. Engrg., 1-1 Hibarigaoka, Tempaku-cho, Toyohashi, Aichi-ken 441-8580 Japan

Severe plastic deformation process using equal channel angular pressing (ECAP) is well-known as an effective technique for improving mechanical properties of bulk-materials. The ultra-fine grained specimens resulting from this process increases remarkably the strength with a fairly good ductility of the materials. Considering perspective of biomedical applications, which needs a biocompatible materials with high strength but kept low modulus, it is interesting to apply such process on the relatively newly developed beta type titanium alloy, Ti-29Nb-13Ta-4.6Zr. This alloy, which is composed of non-toxic and non allergic elements, was found to have low modulus with medium strength, and good biocompability. It is expected to become a potential candidate material for biomedical applications. In this study, rectangular blanks of the alloy with the size of 10x10x85 mm3 were employed by severe plastic deformation process using ECAP with channel intersection angel and channel arch angel are 90° and 20°, respectively. The same process was also performed to other beta-type titanium alloy, Ti-15V-3Cr-3Sn-3Al, for comparison. The change of microstructure and mechanical properties due to the process will be reported.

3:15 PM Break

3:25 PM
Mechanical Properties of Ti-Nb Biomedical Superelastic Alloys Containing Various Ternary Elements: *Tomonari Inamura*[1]; Yusuke Fukui[2]; Hideki Hosoda[1]; Kenji Wakashima[1]; Shuichi Miyazaki[3]; [1]Tokyo Institute of Technology, Precision & Intell. Lab., 4259 Nagatsuta, Midori, Yokohama 226-8503 Japan; [2]Tokyo Institute of Technology, Grad. Student, 4259 Nagatsuta, Midori, Yokohama 226-8503 Japan; [3]University of Tsukuba, Inst. of Matls. Sci., 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8573 Japan

Microstructures and mechanical properties of newly developed Ti-Nb based biomedical superelastic alloys containing various ternary elements such as Al, Ga, In Sn and Ge are characterized in this paper. The alloys were produced by a severe cold-rolling followed by a solution treatment at 1273K. The Ti-Nb-Al alloy exhibited more than 4.5% of superelastic strain, low Young's moduls around 30-40GPa and a high damping capacity. Ti-Nb-Ge alloy exhibited moderate superelasticity and a higher fracture stress. Transmission electron microscopy observation revealed that precipitates are formed in the Ti-Nb-Ge alloy. Well developed recrystallization textures were confirmed by EBSP and XRD pole-figure measurements in all the alloys. The origin of superelastic behavior of the alloys is discussed on the view point of microstructures formed during the thermomechanical treatments.

3:50 PM
Mechanical Properties of Porous Ti-15Mo-5Zr-3Al Compacts Prepared by Powder Sintering: *Naoyuki Nomura*[1]; Takashi Kohama[2]; Shuji Hanada[3]; Akihiko Chiba[1]; Keiichi Sasaki[4]; Masafumi Kanehira[4]; [1]Iwate University, Dept. of Welfare Engrg., 4-3-5 Ueda, Morioka, Iwate 020-0801 Japan; [2]Tohoku University, Grad. Student of Matls. Sci., 2 Aoba, Aramaki, Aoba, Sendai, Miyagi 980-8579 Japan; [3]Tohoku University, Inst. for Matls. Rsch., 2-1-1 Katahira, Aoba, Sendai, Miyagi 980-8577 Japan; [4]Tohoku University, Sch. of Dentistry, 4-1 Seiryo-machi, Aoba-ku, Sendai, Miyagi 980-8575 Japan

In order to improve the strength of porous Ti compacts, porous Ti alloy compacts were fabricated and their microstructure and mechanical properties were investigated in this study. Ti alloy powders were atomized using Plasma Rotating Electrode Process (PREP) with Ti-15Mo-5Zr-3Al (wt.%) bar in an Ar atmosphere. These alloy powders were sintered under 3-30 MPa at 1223K for 7.2 ks by hot pressing (As HP). These compacts were solution treated at 1223 K for 1.2 ks, and then quenched (STQ). X-ray diffraction analysis revealed that a small amount of á phase appeared in â phase in As HP, while there was no á phase in STQ. Young's modulus of STQ is lower than that of As HP by some 5 GPa. It was found that the bend strength of porous Ti-15Mo-5Zr-3Al in the Young's modulus range of human bone is higher than that of porous pure Ti and human cortical bone.

4:15 PM
Development of Mathematical Model for Electrochemical Deoxidation of TiO2: *Pritish Kar*[1]; James W. Evans[1]; [1]University of California, Matls. Sci. & Engrg., 210 Hearst Memorial Mining Bldg., Berkeley, CA 94720-1760 USA

The electrochemical deoxidation (FFC Process) is currently under transformation into commerically viable application at the Titanium Metallurgical Corporation (TIMET). We are developing a Mathematical Model for the same using the classical Newman-Tobias model for a porous electrode as a starting point. The finite element method on FEMLAB is used for the modeling. We will be presenting some of the results of our process and the results indicate the complexities of the process and agree with the experimental results from TIMET.

4:40 PM
Effect of Ta Content on Mechanical Properties of Ti-30Nb-XTa-5Zr: *Nobuhito Sakaguchi*[1]; Mitsuo Niinomi[1]; Toshikazu Akahori[1]; [1]Toyohashi University of Technology, Production Sys. Engrg., 1-1 Hibarigaoka, Tempaku-cho, Toyohashi, Aichi 441-8580 Japan

Ti-Nb-Ta-Zr system alloys such as Ti-29Nb-13Ta-4.6Zr and Ti-35Nb-7Zr-5Ta satisfy the properties demanded for biomaterials. However, there are few reports on the effects of alloying elements on mechanical properties of Ti-Nb-Ta-Zr system alloys. Therefore, in the present study, Ti-30Nb-10Ta-5Zr, which is the simplified compositional alloy of Ti-29Nb-13Ta-4.6Zr for biomedical applications, was fabricated by powder metallurgy. The alloys with Ta content from 0 mass% through 20 mass% were also fabricated. The effect of Ta content on mechanical properties of Ti-30Nb-XTa-5Zr was investigated.

5:05 PM
Electron Beam Casting Technology of Titanium Orthopedic Prosthesis's Production: *S. V. Ladokhin*[1]; N. I. Levitsky[1]; [1]National Academy of Sciences of Ukraine, Physico-Techl. Inst. of Metals & Alloys, 34/1 Vernadsky Ave., Kiev-142 03680 Ukraine

The technology of titanium high precision shaped cast billets manufacture with the use of electron beam melting and casting technique was developed. The new process of EB melting with electromagnetic stirring of melt in skull crucible and casting in chill molds allows obtaining highly refined alloy and minimizing required mechanical operations. Orthopedic prosthesis for the thigh and pelvis bones osteosynthesis in case of proximal bone end fracture, fracture and thigh fracture-dislocation were produced from billets obtained. As an alternative widely used Ti-6Al-4V alloy the composition that includes Mo, Nb and Zr instead V was proposed. The new alloy has higher ultimate tensile strength, yield strength and elongation in comparison with Ti-6-4 one. Implementation of the developed technology of the bioinert alloys cast gives an opportunity to refuse medical alloys import to Ukraine.

Notes

3-Dimensional Materials Science: Computational Methods II

Sponsored by: TMS - Structural Materials Division

Program Organizers: Marc J. De Graef, Carnegie Mellon University, Department Material Science & Engineering, Pittsburgh, PA 15213-3890 USA; Jeff P. Simmons, Air Force Research Laboratory, Materials & Manufacturing Directorate, Dayton, OH 45433 USA; George Spanos, Naval Research Laboratory, Physical Metallurgy Branch, Washington, DC 20375-5000 USA; Jonathan E. Spowart, UES Inc., Dayton, OH 45432 USA

Wednesday AM	Room: Mardi Gras Ballroom F/G
September 29, 2004	Location: Marriott New Orleans Hotel

Session Chairs: Elizabeth A. Holm, Sandia National Laboratories, Dept. 1834, Abuquerque, NM 87185-1411 USA; Andrew B. Geltmacher, Naval Research Laboratory, Code 6350, Washington, DC 20375 USA

8:30 AM Invited

Microstructural Modeling of Phase Transformations: *Jeffrey M. Rickman*[1]; [1]Lehigh University, Dept. of Matls. Sci. & Engrg., 5 E. Packer Ave., Bethlehem, PA 18015 USA

We outline stochastic geometrical methods for modeling first-order phase transformations involving a variety of nucleation and growth scenarios. As a specific example, we consider the catalytic effect of misfit dislocations on the evolution of transformations in thin films. Finally, we discuss simulation strategies for modeling the kinetics and temporal evolution of transformations in 3-dimensional systems using information obtained from 2-dimensional slices.

9:00 AM

Combined 3D Modeling of Solute Diffusion and Grain Boundary Migration in Irregular Cellular Automata: *Koenraad G.F. Janssens*[1]; [1]Sandia National Laboratories, PO Box 5800, MS 1411, Albuquerque, NM 87185-1411 USA

A newly developed, discrete model of three-dimensional, uncoupled, many-element solute diffusion on an irregular grid is presented. The computational model will be presented in detail including examples illustrating the method can be calibrated to real space-time coordinates. Combination of the diffusion model with an earlier developed irregular cellular automaton[1] allows taking into account an evolving solute distribution during the simulation of processes such as grain growth and phase transformation. Examples will be given illustrating the influence of solute drag on different aspects of the microstructure during grain growth. [1]K. G. F. Janssens, "Three Dimensional, Space-Time Coupled Cellular Automata for the Simulation of Recrystallization and Grain Growth", Modelling Simul. Mater. Sci. Eng. (2003) Vol 11 No 2 pp 157-171.

9:20 AM

Computational Investigation on Influences of Initial Microstructures on Three-Dimensional Grain Growth Kinetics: Qiang Yu[1]; *Yujie Wu*[1]; Sven K. Esche[1]; [1]Stevens Institute of Technology, Dept. of Mechl. Engrg., Castle Point on Hudson, Hoboken, NJ 07030 USA

It has been hypothesized that the initial microstructures far away from steady state may result in the slower grain growth observed in isothermal experiments than as is predicted by theories. In this work, various initial microstructures obtained from three-dimensional Cellular Automaton simulations of solidification and static recrystallization were used as input to a Monte Carlo Potts model for grain growth. The simulation results showed that the influences of the initial microstructures on the grain growth kinetics are rather complex. Depending on the nucleation parameters used in the recrystallizaton simulations, the subsequent grain growth exponents varied from the theoretical value to values that indicated fast grain growth. Furthermore, slow grain growth was observed in the simulations starting with columnar initial microstructures obtained from solidification simulations. In addition, rapid grain growth was achieved in the simulations with only a few elongated grains present in the initial microstructures.

9:40 AM Invited

3D Image-Based Modeling of Material Microstructure on the Mesoscale: *Andrew B. Geltmacher*[1]; Alexis C. Lewis[2]; John F. Bingert[3]; [1]Naval Research Laboratory, Code 6350, 4555 Overlook Ave. SW, Washington, DC 20375 USA; [2]National Research Council/Naval Research Laboratory, Code 6350, 4555 Overlook Ave. SW, Washington, DC 20375 USA; [3]Los Alamos National Laboratory, Los Alamos, NM 87545 USA

Mesoscale image-based modeling uses realistic experimentally measured or computationally derived microstructural features to simulate the role of microstructure on the continuum-level response of a material. These models are used to predict the generation of high local stress and strain states that occur through the interaction of microstructural features and the applied loading conditions. 3D image-based models are generated for a superaustenitic stainless steel, from 3D reconstructions using serial sectioning techniques with optical microscopy and electron backscatter diffraction data. These data allow for the incorporation of microstructural features only accessible through the reconstructed microstructures, such as true 3D grain morphology and boundary inclination. The mesoscale image-based models are finite element simulations that use anisotropic elasticity and crystalline plasticity constitutive responses. Additionally, NRL has developed stress-strain visualization techniques that are used to assess the sensitivity of local stress and strain states generated in the simulations from different loading conditions. These techniques highlight critical microstructural features that are likely to initiate failure. We also use the image-based models to simulate the effect of the actual microstructures on their local yielding behavior. The effective 3D yield surface from specific image-based models is calculated using the crystalline plasticity codes.

10:10 AM Break

10:30 AM Invited

Methodologies for Interrogating the Microstructural State of Physical and Virtual Test Specimens: *Matthew P. Miller*[1]; Paul R. Dawson[1]; T.-S. Han[1]; Joel V. Bernier[1]; Jonathan E. Spowart[2]; [1]Cornell University, Sibley Sch. of Mechl. & Aeros. Engrg., 194 Rhodes Hall, Ithaca, NY 14853 USA; [2]UES Inc., AFRL/MLLM Bldg. 655, 2230 Tenth St., Ste. 1, Wright-Patterson AFB, OH 45433 USA

Quantitative characterization experiments can be coupled with microstructure based simulation frameworks to create a means for designing new materials and new material selection methodologies. Comparing simulated to physical results is one of the challenges facing these efforts. For instance, how does one verify that simulated and physical microstructures are statistically identical and how are micromechanical models validated using lattice strain data? This talk focuses on novel methods for experimentally quantifying metallic microstructures and probing both physical and virtual specimens in order to ascertain their microstructural state(s). Two probes are highlighted in this talk - using a model iron-copper two phase alloy. The first is a contiguity probe, which can be used to understand the arrangement of the phases in a multiphase material and the manner in which each phase percolates through the microstructure. Rays are passed through the sample and the line length within each phase determined. In the physical sample, this is accomplished using three dimensional phase maps generated using a unique automated serial sectioning and optical microscopy methodology. Thin layers of material are removed and analyzed with the microstructure reassembled digitally post experimentally. The contiguity probe can then be applied to the reassembled sample. The finite element representation of the alloy is investigated in a similar manner. Rather than a discretization of an image of the sample, the virtual specimen is constructed to be consistent with the various distributions of geometric features most relevant to particular problem. In this case, these are the grain orientation and morphology distributions. The contiguity probe is passed through the virtual sample in a manner similar to that employed on the physical data. The resulting contiguity distribution can then be compared directly to that obtained from the experiment to understand the fidelity in which this attribute of the microstructure was captured in the instantiated sample. A virtual diffraction probe has been constructed to collect crystal strain information from the finite element simulations for comparison to physical in-situ mechanical loading/diffraction (x-ray and neutron) experiments. The crystals that satisfy the Bragg condition are illuminated and the normal strains corresponding to distortions in the crystal lattice normal to a particular set of crystal planes ({hkl}s). In this way the probe mimics the diffraction experiment and diffraction data can be compared directly to the results obtained using the virtual diffraction probe.

11:00 AM Invited

Using Biologically Inspired Computing to Obtain 3D Microstructures: *Elizabeth A. Holm*[1]; David Basanta[2]; Mark A. Miodownik[2]; Peter Bentley[3]; [1]Sandia National Laboratories, Dept. 1834, PO Box 5800, MS 1411, Albuquerque, NM 87185-1411 USA; [2]King's College London, Dept. of Mechl. Engrg., Strand Campus, London WC2R 2LS UK; [3]University College London, Computer Sci. Dept., London UK

Techniques such as serial sectioning and x-ray synchrotron tomography produce three-dimensional (3D) microstructural images that can be used in property and performance models. Our complementary technique creates 3D microstructural images using a Genetic Algorithm to evolve biologically inspired Cellular Automata that self organise into 3D images that are stereologically equivalent to the experimentally measured 2D microstructures provided as inputs. With this approach it is possible to grow 3D microstructures containing particles with different shapes, sizes and interparticle distances using 2D orthogonal images as inputs. While initial calculations are for dispersed particles, the method is general enough that it can be applied to a wide range of microstructures. Some advantages of this technique are that it is fast, does not require specialised or expensive equipment, and requires easily obtained 2D micrographs as inputs. In addition, it can be used to evolve new 3D microstructures based on user created 2D designs.

11:30 AM Invited
Using Three Dimensional Reconstructions to Characterize Coarsening in Toplogically Complex Systems: R. Mendoza[1]; D. Kammer[1]; K. Thornton[1]; *P. W. Voorhees*[1]; [1]Northwestern University, Matls. Sci. & Engrg., 2220 Campus Dr., Cook Hall, Evanston, IL 60208 USA

Three dimensional characterization of a microstructure is needed to understand the coarsening process in systems that possess both positive and negative curvatures. To this end, we have examined the evolution of a dendritic solid-liquid mixture using three-dimensional reconstructions of the microstructure. We show that the morphological evolution of these topologically complex systems during coarsening can be quantified by measuring the probability of finding a patch of interface with a given mean and Gaussian curvature and is predicted by the flow in this curvature space that is induced by the coarsening process. We measure the anisotropy of the microstructure using the probability of finding a normal of a given direction. We find that the anisotropy of the microstructure changes with time during coarsening. Finally, we have measured the evolution of the genus of the microstructure as a function of time during coarsening.

Advancements in Mechanical Property Characterization at the Micro- and Nano-Scale: Modeling, Simulation, and Experimental Observations of Dimensional Size Effects

Sponsored by: TMS - Structural Materials Division
Program Organizers: Mike Uchic, Air Force Research Laboratory, Dayton, OH 45433-7817 USA; Kevin J. Hemker, Johns Hopkins University, Department of Mechanical Engineering, Baltimore, MD 21218 USA; Marc Zupan, University of Maryland, Baltimore, MD 21250 USA

Wednesday AM — Room: Mardi Gras Ballroom B
September 29, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Michael J. Mills, Ohio State Univeristy, Dept. of Matls. Sci. & Engrg., Columbus, OH 43210 USA; Taher A. Saif, University of Illinois, Dept. of Mechl. & Indust. Engrg., Urbana, IL 61801 USA

8:30 AM Invited
Discrete Dislocation Modeling of Plastic Deformation in Small Volumes: *Alan Needleman*[1]; E. Van der Giessen[2]; [1]Brown University, Mech. of Solids & Struct., 182 Hope St., Providence, RI 02912 USA; [2]University of Groningen, Dept. of Applied Physics, Groningen NL-9747 Netherlands

There is considerable experimental evidence that plastic flow in crystalline materials is size dependent over length scales of the order of tens of microns and smaller. This size dependence arises in a variety of contexts; e.g. micro- and nano- indentation and the thermo-mechanical response of thin films. One well-appreciated origin of size effects is associated with imposed plastic strain gradients and geometrically necessary dislocations. In addition, strain gradients and boundary layers leading to size-dependent response can occur in circumstances where, at least in principle, a more or less homogeneous response is possible but where the physics of dislocation motion prevents it. Furthermore, in small volumes plastic flow can be source limited. Discrete dislocation analyses of various plastic flow processes will be used to illustrate a range of size effects and their implications for deformation and fracture.

9:00 AM
Atomistic-Based Continuum Modeling of Deformation in Nanocrystalline Copper: *Derek Hunter Warner*[1]; Jean-Francois Molinari[1]; [1]Johns Hopkins University, Dept. of Mechl. Engrg., 3400 N. Charles St., Baltimore, MD 21218 USA

This work focuses on the development of a 2D continuum model which explicitly incorporates the deformation mechanisms present in nanocrystalline metals. By using previous atomistic calculations that examined the behavior of several tilt grain boundaries under an applied load, constitutive laws were developed that were input into the finite element calculation. An application specific, contact/adhesion algorithm was developed to account for grain boundary sliding. Direct observation of the microstructure throughout its deformation evolution yielded useful insights pertaining to the collective deformation mechanisms present in granular materials. Additionally, parametric studies were performed correlating mechanical response with structural variables of the microstructure such as grain size distribution and orientation.

9:20 AM
Experimental Techniques for Uncovering Deformation Mechanisms in Nanocrystalline Al Thin Films: *Daniel Santiago Gianola*[1]; Kevin J. Hemker[1]; William N. Sharpe[1]; [1]Johns Hopkins University, Dept. of Mechl. Engrg., 3400 N. Charles St., Baltimore, MD 21218 USA

Nanocrystalline materials have received considerable interest due to deviations in mechanical properties in comparison to their coarse-grained counterparts. Molecular dynamics and direct transmission electron microscopy studies have evidenced an apparent change in the underlying mechanism that controls plastic deformation in materials with grain sizes that are less than ~50 nm, in which a transition occurs from normal dislocation slip to grain boundary sliding and partial dislocation activity. Attempts to characterize the mechanisms that govern the mechanical response are inhibited by the challenges associated with direct mechanical testing of submicron thin films. To link these nanoscale mechanisms with macroscale responses, a unique microsample testing apparatus is utilized to test submicron thin films using various testing modalities. Two types of nanocrystalline thin film specimens, fabricated using MEMS inspired processes such as photolithography and bulk micromachining, and testing techniques have been developed and will be discussed. Standard uniaxial tensile tests are performed to measure conventional properties, while transient experiments (e.g. stress relaxation, strain-rate change) are employed to identify the mechanisms that drive the material response.

9:40 AM Invited
Discrete Dislocation Plasticity Analysis of Static Friction and Surface Contact: *V. S. Deshpande*[1]; A. Needleman[2]; Y. F. Gao[2]; A. F. Bower[2]; E. Van der Giessen[3]; [1]Cambridge University, Dept. of Engrg., Trumpington St., Cambridge CB2 1PZ UK; [2]Brown University, Mech. of Solids & Struct., 182 Hope St., Providence, RI 02912 USA; [3]University of Groningen, Dept. of Applied Physics, Groningen 9747 AG Netherlands

Predicting the effective frictional resistance of solid surfaces in contact involves two distinct issues: (i) determining the resistance to sliding at a single contact and (ii) determining the actual area of contact due to contact of asperities. Here we present a discrete dislocation plasticity analyses of these issues. First we analyse the shear stress needed to initiate sliding between a flat indenter and a single crystal substrate. Plastic deformation in the substrate is modelled using discrete dislocation plasticity while the adhesion between the indenter and the substrate is characterised by a shear traction versus sliding displacement cohesive relation. The results show that for sufficiently small contact sizes adhesion dominates and the friction stress is equal to the cohesive strength, while for sufficiently large contacts plasticity dominates and the friction stress is approximately equal to the flow strength. For intermediate contact sizes, the friction stress is contact-size dependent. Results are presented that show the effects of superposed normal pressure, of cohesive strength and of dislocation source density on the value of the friction stress and its size-dependence. Next, with the aim of predicting the actual area of contact, we investigate contact between a rigid platen with a sinusoidal profile and a flat single crystal substrate. This serves as a unit process for contact between surfaces whose roughness is idealised with a Weierstrass profile. Relations between contact pressure and contact size are developed. Size effects arising from source limited plasticity and from the interaction of neighbouring asperities are discussed.

10:10 AM Break

10:30 AM Invited
Mechanics of Freestanding Submicron Thin Films-Size Scale Plasticity and Fracture: *Horacio Espinosa*[1]; [1]Northwestern University, Dept. of Mechl. Engrg., Evanston, IL 60208 USA

Over the past decade, there has been a substantial thrust to reduce the size of electronic and electromechanical systems to the micron and submicron scale by fabricating devices out of thin film materials. In these applications, successful device development requires a thorough understanding of material mechanical properties as a function of device characteristic dimension. At this scale, specimen geometry and dimensions are similar in size to the material microstructural features. Consequently, new tests and models capable of accurately capturing this effect are highly needed. In this presentation, a new on-chip membrane deflection experiment specially designed to investigate material elastic behavior (including grain anisotropy and morphological effects), plasticity (including size effects in the submicron regime), and fracture will be discussed. Two examples of research recently conducted at Northwestern University will be presented. The first example examines plasticity size effects in freestanding fcc thin films in the absence of macroscopic strain gradients. Experimental results including transmission electron microscopy will be presented to demonstrate that indeed strong plasticity size effects exist and to highlight their possible sources. Current shortcomings of plasticity theories at the submicron scale and its implication in the design of micro/nano devices will be discussed. The second example involves the identification of elasticity, strength and fracture properties of ultra-nano-crystalline diamond, a new material poised to impact the development of novel micro and nano-electro-mechanical systems.

11:00 AM
Exploring External Size Effects in Crystal Plasticity: *Dennis M. Dimiduk*[1]; Michael D. Uchic[1]; Triplicane A. Parthasarathy[2]; [1]Air Force Research Laboratory, Matls. & Mfg. Direct., AFRL/MLLM, Wright Patterson AFB, OH 45433-7817 USA; [2]UES, Inc., 4401 Dayton-Xenia Rd., Dayton, OH 45432 USA

Size scales in crystal plasticity—length scales associated with dislocation nucleation, motion, and substructure evolution—greatly influence flow stresses and strain-hardening rates during plastic deformation. We have used micro-scale fabrication methods and a readily-interpretable test technology to systematically explore external size-scale effects in a variety of metallic alloys. In particular, we have examined single crystals of three fundamentally unique types of metals, and a nanocrystalline metal. The results show that the sample dimensions at the micron-size scale can dramatically affect the mechanical properties of a deforming volume. This talk will focus on understanding how sample size can limit the length scales available for plastic processes. Importantly, the results emphasize that at the micron-size scale one must define both the external geometry and the internal structure in order to characterize the mechanical response of a material.

11:20 AM
Ultra Small-Scale Mechanical Testing of Ti-6Al: *S. J. Polasik*[1]; H. L. Fraser[1]; M. J. Mills[1]; M. D. Uchic[2]; D. M. Dimiduk[2]; [1]Ohio State University, Matls. Sci. & Engrg. Dept., Columbus, OH 43210 USA; [2]Air Force Research Laboratory, Matls. & Mfg. Direct., Wright-Patterson AFB, OH 45433-7817 USA

In order to alleviate the need to grow macroscopic single crystal specimen to determine the mechanical behavior of individual grains and other microconstituents within engineering alloys, a testing methodology capable of deforming small volumes of material has been developed. A Dual Beam Focused Ion Beam (DB-FIB) microscope is used to site-specifically machines cylindrical compression specimen with a L/D ratio of 2 and diameters ranging from 5μm to 40μm. A nanoindenter equipped with a flat-ended tip is then used to compress the specimen in uniaxial compression at room temperature. Currently, single crystal compression samples of Ti-6Al oriented for basal slip are under investigation as a model of the α-phase of commercial Ti alloys. The combination of TEM foil preparation and micromanipulation within the DB-FIB facilitates the examination of the effect of size on the deformation processes as compared to the bulk behavior.

Applications of Orientation Microscopy Techniques to Phase Transformations: Emerging Techniques and Applications

Sponsored by: TMS - Materials Processing & Manufacturing Division, TMS - MPMD-Phase Transformations Committee-(Jt. ASM-MSCTS)
Program Organizers: Robert E. Hackenberg, Los Alamos National Laboratory, Materials Science and Technology Division, Los Alamos, NM 87545 USA; Richard W. Fonda, Naval Research Laboratory, Washington, DC 20375 USA; Milo V. Kral, University of Canterbury, Department of Mechanical Engineering, Christchurch New Zealand

Wednesday AM — Room: Mardi Gras Ballroom C
September 29, 2004 — Location: Marriott New Orleans Hotel

Session Chair: Milo V. Kral, University of Canterbury, Dept. of Mechl. Engrg., Christchurch New Zealand

8:30 AM Invited
Impact of EBSD on the Development of a Gd Containing Alloy for Spent Nuclear Fuel Applications: *Joseph R. Michael*[1]; Charles V. Robino[1]; John N. Dupont[2]; Ron E. Mizia[3]; [1]Sandia National Laboratories, PO Box 5800, MS 0886, Albuquerque, NM 87185-0886 USA; [2]Lehigh University, Matls. Sci. & Engrg., 5 E. Packer Ave., Bethlehem, PA 18015 USA; [3]Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID USA

Gd enriched alloys are currently being considered for structural neutron shielding in long-term containment vessels for spent nuclear fuel storage. Initial studies were focused on the development of a 316 stainless-based matrix with added Gd. These materials were found to have very limited hot ductility. Phase identification using EBSD played an important role in the understanding of the severe limitations of these alloys resulting from the solidification behavior. To overcome these difficulties, Ni-based alloys with added Gd are currently being developed. EBSD has been important to the effort through both phase identification and orientation mapping of the resulting multiphase microstructures. Unique laboratory deformation samples, coupled with EBSD assessments of microstructural evolution have been used to determine appropriate processing routes to produce these alloys with suitable properties. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United Stated Department of Energy (DOE) under contract DE-AC0494AL85000.

9:00 AM
Phase Differentiation Reliability in Automated Electron Backscatter Diffraction: *Stuart I. Wright*[1]; Matthew M. Nowell[1]; [1]EDAX, TSL, 392 E. 12300 S., Draper, UT 84020 USA

Automated Electron Backscatter Diffraction (EBSD) or Orientation Imaging Microscopy is well suited for investigating orientation relationships between phases. In studying phase transformations, the chemical compositions between the parent and child phases are typically quite similar, if not identical (i.e. austenite and ferrite) but are dissimilar crystallographically. EBSD is well suited to automatically differentiating such phases. However, many of the phases considered in phase transformation studies are also similar or identical crystallographically (i.e. austenite and martensite). In these cases, post-processing techniques must be used to differentiate between phases. This presentation will examine novel techniques used to differentiate phases both during the collection of EBSD data as well as after a set of EBSD data has been collected. Methodologies for predicting the reliability of the phase differentiation procedure during data collection will be presented.

9:25 AM
On the Potential of 3D X-Ray Diffraction Microscopy to Study Solid State Phase-Transformations: *Erik Mejdal Lauridsen*[1]; Richard Fonda[2]; George Spanos[2]; [1]Risø National Laboratory, Ctr. for Fundamental Rsch., Metal Struct. in Four Dimensions, Frederiksborgvej 399, Roskilde 4000 Denmark; [2]Naval Research Laboratory, Physl. Metall. Branch, Washington, DC 20375 USA

3D X-ray diffraction (3DXRD) microscopy is an emerging new technique based on diffraction of high energy (> 50 keV) synchrotron radiation for 3D/4D characterization of microstructures in metals and other poly-crystalline materials. Due to the high penetration power and non-destructive nature of high energy x-rays, 3DXRD microscopy enables unique in-situ observations of individual bulk grains during e.g. heating and/or deformation. The presentation will include an introduction to the 3DXRD microscopy technique, with an overview of the available operation modes and their potential for the study of phase-transformations. Special emphasis will be on measurements of 3D/4D grains maps utilizing diffraction based reconstruction algorithms.

9:50 AM
Investigation of Corrosion Behavior and Microstructure of Zircaloy-4 Irradiated by High Doses of Ar and Kr Ions: Qian Wan[1]; Xinde Bai[1]; Xiaoyang Liu[1]; [1]Tsinghua University, Dept. of Matls. Sci. & Engrg., Beijing 100084 China

In order to investigate the ion irradiation effect on the corrosion behavior and microstructure of Zircaloy-4, Zircaloy-4 specimens were irradiated by Ar and Kr ions using an accelerator at an energy of 300 keV, with the dose from 1e15 to 1e17 ions/cm2. Post-irradiation corrosion tests were conducted to rank the corrosion resistance of the resulting specimens by potentiodynamic polarization curve measurements. The vacancy profile induced by Ar ion irradiation was calculated using Monte Carlo simulation program SRIM 96, and measured by means of slow positron annihilation spectroscopy (SPAS). The microstructures of the irradiated surface were examined using Glancing Angle X-ray Diffraction (GAXRD). The potentiodynamic tests showed that as the irradiation dose increased, the passive current density first decreased and subsequently increased. The mechanism of the corrosion behavior transformation was due to amorphous phase formation followed by recrystallization of the irradiated surface.

10:15 AM Break

10:35 AM
Combined EBSD and CSLM Study of Surface Oxidation in Si/Al TRIP Steels: *C. Thorning*[1]; S. Sridhar[1]; D. M. Haezebrouck[2]; T. Simpson[3]; [1]Carnegie Mellon University, Dept. of Matls. Sci. & Engrg., 5000 Forbes Ave., Pittsburgh, PA 15232 USA; [2]US-Steel Technical Center, Monroeville, PA 15146 USA; [3]ISG Research, Bethlehem, PA 18015 USA

The crystallography of a cold rolled and annealed Si/Al TRIP steel was characterized using EBSD. The sample was subsequently heated in a controlled atmosphere and SiO_2 growth on the surface of the sample was studied using confocal scanning laser microscopy (CSLM). The crystal orientation maps and CSLM recordings were combined to provide real-time observation of oxide nucleation and growth as related to surface crystallography. Combining EBSD and CSLM studies, the crystallographic basis of surface phase transformations may be understood.

11:00 AM

A Study of Austenite Decomposition Combining Direct Visualization Through Confocal Microscopy and Orientation Imaging: *Eric D. Schmidt*[1]; S. Sridhar[1]; [1]Carnegie Mellon University, Dept. of Matls. Sci. & Engrg., 5000 Forbes Ave., Pittsburgh, PA 15213 USA

Although the microstructure of steels have been studied following a wide range of heat treatments, most of the understanding is limited to a posteriori characterization techniques. A hot-stage confocal scanning laser microscope has been used to observe these transformations in situ. Orientation imagery can relate growth rates and morphologies to crystallographic orientation. Given the limited growth directions in which these transformations can occur, a good approximation of the 3D growth rate can be calculated using the surface component of growth. Orientation images also show that allotriomorphs nucleate at austenite grain boundaries and groups of parallel widmanstätten laths nucleate on allotriomorphs with the same orientation as the parent allotriomorph. These observations suggest that widmanstätten ferrite is the manifestation of stable perturbations on a planar allotriomophic ferrite/austenite interface. Results are discussed in light of transformation models based on diffusion, heat transfer, lattice strain, and nucleation kinetics.

11:25 AM

In-Situ Studies of Widmanstätten Ferrite Plate Nucleation and Growth in Fe-C Alloys: *Dominic Joseph Phelan*[1]; Rian Johannes Dippenaar[1]; [1]University of Wollongong, Steel Inst., Northfields Ave., Wollongong, NSW 2500 Australia

Experimental and analytical studies are underway to probe Widmanstätten ferrite plate nucleation and growth phenomena in Fe-C alloys. In-situ observations were conducted using Laser Scanning Confocal Microscopy (LSCM) in a concentric solidification arrangement. A unique microstructure develops where-by Widmanstätten ferrite plates are engulfed by pearlite at a number of stages. A Focused Ion Beam (FIB) milling and imaging technique has been utilised to probe microstructural and crystallographic aspects of nucleation and growth of the engulfed plates.

Development and Application of Hot Rolled Flat Products: Session I

Sponsored by: AIST, AIST - Division V, AIST - Division VI, AIST - Division VII

Program Organizers: Mark R. Blankenau, SeverStal NA, Dearborn, MI 48121 USA; Brian J. Allen, AK Steel Corp., Middletown, OH 45043 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Wednesday AM Room: La Galerie 3
September 29, 2004 Location: Marriott New Orleans Hotel

Session Chair: Matt S. Walp, DaimlerChrysler, Matls. Engrg., Auburn Hills, MI 48326 USA

8:30 AM

Strain Induced Precipitation During Hot Deformation in HSLA Steels - Effect of Vanadium Supersaturation in Austenite: *Cheng Ai Khoo*[1]; George Fourlaris[1]; [1]University of Wales, Matls. Rsch. Ctr., Singleton Park, Swansea SA2 8PP UK

V additions are known to have a profound effect on the metallurgical characteristics of austenite during hot deformation. During a hot deformation sequence the recrystallisation stop temperature (TRST) appears to be the dominant factor since below the TRST fully non-recrystallised austenite grains are present, while above fully or partially recrystallised grains are present. In a hot deformation experiment parameters such as the amount of strain, strain rate, and amount of solute supersaturation of the microalloy addition control the recrystallisation stop temperature (TRST). From a commercial processing viewpoint, knowledge of where the TRST lies in relation to the deformation temperatures employed for the finishing passes is essential in achieving equiaxed and fine microstructures. Consequently, this study develops techniques which would allow for the accurate measurement of V in solution in austenite, as a function of both reheat and deformation temperature, relevant to conditions of hot working employed during industrial practices.

9:00 AM

Some Physical Metallurgy Aspects of High Strength Hot-Rolled Cb-Ti Microalloyed Steels with Superior Fracture Resistance and Formability: *Harish Nathani*[1]; Devesh K. Misra[1]; Jack E. Hartmann[2]; Fulvio Siciliano[3]; Tadeu Carneiro[3]; [1]University of Louisiana, Matls. Sci. & Engrg. Grp., Dept. of Chem. Engrg., Rex Dr., Madison Hall 217F, Lafayette, LA 70503 USA; [2]International Steel Group, Indiana Harbor Works, 3001 Dickey Rd., E. Chicago, IN 46312 USA; [3]Reference Metals Company, 1000 Old Pond Rd., Bridgeville, PA 15017 USA

Columbium-titanium microalloying approach was used to process hot-rolled microalloyed steels of yield strength 420-770 MPa. Ferrite microstructure was the basis for processing lower yield strength 420-630 grades, while ferrite-bainite was for the ultra-high strength 690-770 MPa grades. The elements preferred to obtain bainite were boron and molybdenum. Additionally, it is important to control the effective Cb by control of the C, N and the Ti/N ratio to obtain the required high strength together with toughness. The superior fracture resistance and edge formability of steels is attributed to cumulative contribution of fine grain size and high intensity of the desired {332}<113> texture. These characteristics add to the benefits derived from the bainitic constituent in ultrahigh strength 690-770 MPa grades.

9:30 AM

Microstructure Evolution During Thermomechanical Testing in Novel IF Strip Steels: *Sara Louise Porter*[1]; George Fourlaris[1]; [1]University of Wales, Matls. Rsch. Ctr., Sch. of Engrg., Swansea SA2 8PP UK

The technological parameters of hot rolling of strip steels, directly influence the microstructure and hence the mechanical properties of the hot rolled steel. A series of thermo-mechanical simulations of the hot rolling process have been carried out using the Gleeble 3500 unit. The equipment was used to simulate the hot rolling conditions of the hot mill such as the slab reheat temperature, roughing temperature and deformation, finishing temperature and deformations, controlled cooling on the run-out table and the cooling from the coiling temperature. The final stage of the simulation is the slow cooling of the coil to ambient temperature. The aim was to investigate the effect of these parameters on the microstructure of the two novel IF steel grades, a Ti only and a mild Ti-Nb grade. The microstructures obtained were characterised using optical and electron microscopy techniques. Microstructural prediction permits the optimisation of processing routes followed in industrial practice and leads to the development of strip steel products with modified mechanical property characteristics.

10:00 AM Break

10:30 AM

Recent Steel Developments in the Integrated Technology of CSP: *Carl-Peter Reip*[1]; Christian Bilgen[1]; Christian Geerkens[1]; Wolfgang Hennig[1]; Ingo Schuster[1]; [1]SMS Demag AG, Eduard-Schloemann-Str. 4, Düsseldorf 40237 Germany

The Compact Strip Production (CSP) represents a highly developed technical process, offering nowadays the production of hot strip at low production costs. Due to the high productivity and the outstanding product quality the CSP technology accounts for a capacity of more than 40 million t/a. The product range has been continuously extended during the past 15 years, now ranging from low- and medium-carbon grades to stainless ferritic and austenitic qualities as well as grain-oriented Si steels. Furthermore, the production of hot-rolled strip with a multiphase microstructure for automotive application and of hot strip for welded line pipes is considered to be a major challenge not only by CSP hot strip producers. The paper particularly highlights the most important recent steel developments. Additionally, the special features of the CSP technology in the areas of casting, direct charging, rolling and cooling with respect to the final hot strip properties are discussed.

11:00 AM

Loop Sensor for Hot Strip Mill in Steel Rolling Process: *A. K. Paul*[1]; K. N. Rao[1]; B. K. Santra[1]; N. Neogi[1]; [1]Steel Authority of India Limited, R&D Ctr. for Iron & Steel, Post - Doranda, Ranchi 834002 India

In a Hot Strip Mill, control of looper angle is very important to maintain a definite tension between two successive stands for stable rolling operation. The final dimension of the rolled product depends on the accuracy and the transient response of the looper angle control system. The goal of this research work is to provide stability of the finisher by fast acting controller and intelligent sensor. An absolute encoder based looper angle sensor has been developed around a microcontroller (89C52), which provides an intelligent output to the stand speed drive and looper motor drive. The transfer function of the sensor can be modified to meet the process demand. The sensor has been installed in such a way that the jerking load is avoided in the sensor. The scheme has been implemented in Hot Strip Mill of Rourkela Steel Plant, India. Implementation of this scheme has resulted in reduction in cobble by 66%, and reduction in mill delay by 55%.

11:30 AM
Galvanizing of High Strength Hot Rolled Steels: *Benoit Voyzelle*[1]; Sylvie Dionne[1]; Elhachmi Essadiqi[1]; Éric Baril[2]; Joseph R. McDermid[3]; Frank Goodwin[4]; [1]Materials Technology Laboratory, 568 Booth St., Ottawa, Ontario K1A 0G1 Canada; [2]Noranda Inc., 2250 Alfred Nobel Blvd., Ste. 300, Ville St-Laurent, Québec H4S 2C9 Canada; [3]McMaster University, Dept. of Mechl. Engrg., 1280 Main St. W., Hamilton, Ontario L8S 4L7 Canada; [4]International Lead Zinc Research Organization, Rsch. Triangle Park, NC 27709-2036 USA

High strength hot rolled steel grades are attractive to the automotive industry because of their potential for reducing vehicle weight and overall materials costs. This paper presents the results of laboratory scale research to develop a galvanizing process window for selected precipitation-strengthened hot rolled steels. The galvanizing behavior was characterized as a function of reheating temperature, hydrogen content and dew point. Conditions were identified which produced good quality coatings on the hot rolled substrates while maintaining the target yield strength of 500-550 MPa and 20-25% total elongation.

12:00 PM
The Analysis of Relations Between Filar Spot Stain of Electro Galvanized Antifinger Plate and the GOSS Texture of Hot Strip: *Fabing Wen*[1]; [1]Baosteel, Hot Rolling Mill Plant, Shanghai 200941 China

There was filar spot stain on the electro-galvanized antifinger plate. This paper introduces the two reasons that cause the defect. One is the Goss texture formed on the surface of the hot rolling strip which leads to the mirroring phenomenon after the strip is galvanized. Its color is different with the color of other parts surrounding. The other reason is missing galvanizing on the cold sheet. Why the Goss texture formed during hot rolling process is analyzed mainly based on the fact producing data and theory in this paper, such as the coefficient of friction between strip and roll, the finishing temperature of strip and so on. The method that can decrease the formation of Goss texture is put forward as well.

Engineered Steel Surfaces: Nanotechnology, Hardness, Wear Resistance

Sponsored by: AIST, TMS, AIST - Division VI, TMS - SMD-Corrosion and Environmental Effects Committee-(Jt. ASM-MSCTS)
Program Organizers: Bruce Kukuch, Ispat Inland Steel R&D, Coatings and Surface Technology, East Chicago, IN 46312 USA; Raúl B. Rebak, Lawrence Livermore National Laboratory, Livermore, CA 94550 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Wednesday AM — Room: Grand Ballroom L
September 29, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: James Maloney, The Timken Company, Adv. Matls. R&D, Canton, OH 44706 USA; Bruce Kukuch, Ispat Inland Steel R&D, Coatings & Surface Tech., E. Chicago, IN 46312 USA

8:30 AM
Surface Hardening of Austenitic Steels by Low Temperature Colossal Supersaturation: *Gary M. Michal*[1]; Frank Ernst[1]; Yan Cao[1]; [1]Case Western Reserve University, Matls. Sci. & Engrg., 10900 Euclid Ave., Cleveland, OH 44106-7204 USA

A new approach has been applied to harden the surface of austenitic steels. Gas phase carburization treatments have been carried out below 500 C. At such low temperatures the precipitation of carbides can be kinetically suppressed enabling the creation of colossal supersaturations of interstitial carbon. Surface hardness levels approaching 1200 HV25 have been achieved in 316 stainless steel while maintaining an alloy comprised of single phase austenite. Compressive residual stresses of 2 GPa and enhanced corrosion resistance also are produced. Potential applications of colossal supersaturation surface hardening to a range of austenitic steel alloys will be discussed.

8:55 AM
Improvement of Hardness and Wear Resistance in Stainless-Steel-Base Surface Composites Fabricated by High-Energy Electron-Beam Irradiation: *Kyuhong Lee*[1]; Eunsub Yun[1]; Sunghak Lee[1]; Nack Jun Kim[1]; [1]Postech, Advd. Matl. Sci. & Engrg., San 31, Namgu Hyojadong, Pohang, Kyungbuk 790-784 S. Korea

Stainless-steel-based surface composites reinforced with TiC and SiC were fabricated by high-energy electron beam irradiation. Four kinds of powder/flux mixtures, i.e., TiC, (Ti+C), SiC, and (Ti+SiC) powders with 40 wt.% of CaF2 flux, were deposited evenly on an AISI 304 stainless steel substrate, which was irradiated with an electron beam. In the composite layer fabricated with Ti and C powders, a number of primary TiC carbides were precipitated without TiC agglomerates or pores. This indicated more effective TiC precipitation obtained from the melting of Ti and C powders, instead of TiC powders. A large amount of precipitates such as TiC and Cr7C3 improved the hardness, high-temperature hardness, and wear resistance of the surface composite layer two or three times greater than that of the substrate. In particular, the surface composite fabricated with SiC powders had the highest volume fraction of Cr7C3, and thus showed the best hardness, high-temperature hardness, and wear resistance.

9:20 AM
A Complete Study on the Electroless Ni-P-PTFE Composite Coatings: *Mehran Haratian*[1]; Maryam Marandian[1]; Seyed Mahmoud[2]; [1]Iran International Engineering Company(IRITEC), Eng. Mehran Haratian, No. 21/23, Khodami(Bijan)St.,Vanak Sq., Tehran Iran; [2]Isfahan University of Technology

In recent years most commercial interests have focused on electroless Ni-P- PTFE composite coatings for applications including valves, carburetor components, pump rotors, nuts and bolts, etc. This paper reports a complete study on electroless Ni-P-PTFE composite coatings. The steps in making a properly operating electroless composite plating bath are described. The effects of surfactant type and concentration on electroless Ni-P-PTFE deposition rate were investigated, showing that increasing the surfactant and PTFE concentration reduces deposition rate. SEM, XRD, dot mapping, and optical microscopy were used to define the ratio that described the optimum conditions of deposition. Wear and tribological behavior of the coatings were examined, focusing on the effect of key factors such as heat treatment of the deposits, amount of PTFE codeposited in the films, and load. Wear and frictional behavior of coatings are described through graphs of weight loss and coefficient of friction against wear distance. The most wear resistant coating is identified. Also presented are the effects of heat treatment, deposit thickness and amount of PTFE particles in the film on the hardness of deposits. It was determined that increasing the amount of PTFE in deposits meant reduction of hardness in the coatings, and that maximum hardness of coatings was obtained when deposits were heat treated at 400 C for 1 hour.

9:45 AM
Characteristic Features of Cutaneous Layer of Burnished Surfaces: *V. S.R. Murti*[1]; K. Sudhakar[2]; [1]Osmania University, Dept. of Mech. Engrg., Hyderabad 500 007 India; [2]Government Polytechnic, Mech. Engrg. Dept., Mahabua Nagar 509 001 India

Burnishing improves surface texture by flattening of surface roughness aspirates through compression by a hard roller or ball. The associated mechanism is characteristically defined as cold working of roughness peaks and simultaneous swelling of flanks of the corresponding valleys. The resulting surface exhibits highly improved surface texture, micro hardness and compressive residual stresses that further contribute to high fatigue strength. The present studies present the experimental results from ball and roller burnishing of cylindrical surfaces which include scanning electron microscopy, Vicker's micro hardness and X-Ray Diffraction analysis of residual stresses. The results are even better with twin pass burnishing employing reversal of feed direction of the burnishing tool in the subsequent pass.

10:10 AM Break

10:20 AM
Surface Modification of 4340 Steel with Iron-Aluminides Using High-Energy Density Processes: *Govindarajan Muralidharan*[1]; Narendra B. Dahotre[2]; Craig A. Blue[1]; Vinod K. Sikka[1]; [1]Oak Ridge National Laboratory, Metals & Ceram., Bldg. 4508, MS-6083, 1 Bethel Valley Rd., Oak Ridge, TN 37831-6083 USA; [2]University of Tennessee, Dept. of Matls. Sci. & Engrg., 326 Dougherty Hall, Knoxville, TN 37996 USA

Iron aluminides possess several attractive properties motivating significant research and development efforts over the past years. Fe_3Al and FeAl show excellent resistance to oxidation and sulfidation in aggressive environments. Due to their excellent properties and cost considerations, appropriate compositions of iron aluminides could find applications as coatings on more traditional higher-strength materials with inferior corrosion-resistant properties at higher temperatures. Other experiments with bulk iron aluminides have shown that they have superior wetting characteristics with hard particles such as TiB_2. Iron aluminide coatings reinforced with hard, wear-resistant TiB_2 particles could potentially possess a combination of superior oxidation/sulfidation properties along with excellent wear-resistance. In this work, we present some of the results of our efforts to coat a representative steel, 4340, with iron-aluminides using a high-powered laser and a high-density infrared lamp. Particular emphasis will be placed on the relationship between structure and composition of the coatings, their properties, and processing parameters.

10:45 AM
Engineered Surfaces for Steel Rolling Element Bearings and Gears: Ryan D. Evans[1]; Carl R. Ribaudo[1]; Gary L. Doll[1]; Elizabeth P. Cooke[1]; *James L. Maloney*[1]; [1]The Timken Company, Advd. Matls., MC RES 13, PO Box 6930, Canton, OH 44706 USA

Engineered Surfaces (ES) is an emerging technology area that covers the selection and application of advanced topographical modifications and thin film coatings to improve the tribological performance of precision mechanical systems without component redesign. Surface damage and wear in complex mechanical systems can be reduced with ES technologies, leading to improved performance and longer service lives. Representative ES topographical modification (TM) and thin film coating technologies are introduced and followed by test data demonstrating their use on steel rolling element bearings and gears. For example, composite coatings consisting of nanometer-sized metal carbide crystals embedded in an amorphous hydrocarbon matrix are used in tapered roller bearings to prolong fatigue life, inhibit rib-roller end scuffing, and provide protection against false brinelling. Combinations of TM and these coatings have also increased the scuffing resistance of gears in tests.

11:10 AM
Rheological Modeling of Fracture Mechanics Between Hard and Soft Coatings: *Maksim V. Kireitseu*[1]; [1]Institute of Mechanics and Machine Reliability, Lesnoe 19 - 62, Minsk 223052 Belarus

The present work describes rheological modeling of novel nanostructured coatings (chrome carbide nanoparticles/aluminum oxide/ soft aluminum substrate) and (steel/viscous-elastic stressed polymer/aluminum/aluminum oxide) at Hertzian indentation. When the hard aluminum oxide-based coatings are brought into contact with a ceramic or a metal indenter, different stress-deformation modes can be developed between the materials. Strains and forces will depend upon the state of the surface, its roughness, and the fundamental mechanical properties of the two solids (indenter and substrate). Mechanical behavior between the coatings and another solid indenter are discussed from a theoretical consideration of the mechanical constants (elasticity, plasticity and viscosity) of the coatings and experimentally by relating loading forces and stresses to the interface resulting from the contact. Rheological models proposed for the coatings were confirmed by in-situ experiments using principal Hertzian theory. Experimental evidence showed good agreement between the models and mechanical behavior of the coatings. Load rating tests revealed ultimate stresses and stress-deformation modes for both the coatings and their particular layers. The models and their behavior under a few fundamental conditions of loading (triangle, pulse, sinusoidal etc.) are discussed.

11:35 AM
The Microstructure and Properties of Nano Multi-Coatings: *Xiying Zhou*[1]; Wensong Lin[1]; Shiqiang Qian[1]; [1]Shanghai University of Engineering and Science, Sch. of Matls. Sci. & Engrg., Shanghai 200336 China

Different composite nickel matrix multi-coatings containing various nano-powders (Al2O3/AlSiO2/AlZrO2) were fabricated by electro-brush plating, using electro-brush solutions created by employing different nano-powders and dispersing methods. The surface morphology and microstructure of coatings were observed by means of S-2700 SEM. Microhardness at room temperature and higher temperatures (100 / 600C) and wear resistance of coatings were analyzed. The scratch tester was used to investigate friction coefficients of coatings. The results showed that the microstructure of multi-coatings was obviously finer compared to the coating without nano-powders. During the formation of multi-coatings, a small part of nano-powders are thought to provide a surface that promotes the nucleation of the coatings. So, the growth of grain size of microstructure is limited. Micro-hardness increased as much as 30% with increase of nano-powder content in electro-brush plating solution. The wear resistance and micro-hardness after heating to high temperature was also improved. The strengthening effects differed with different kinds of nano-powders. This is due to the combination of dispersion strengthening and grain size strengthening. Friction coefficients of multi-coatings are slightly reduced. Based on these results, the mechanics of nano multi-coatings are discussed in detail.

Materials Damage Prognosis: Local and Global Methods and Sensors for Interrogation of Materials Damage State I

Sponsored by: TMS - Structural Materials Division
Program Organizers: James M. Larsen, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson AFB, OH 45433-7817 USA; Jeffrey R. Calcaterra, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson Air Force Base, OH 45433-7817 USA; Leo Christodoulou, Defense Advanced Research Agency, Arlington, VA 22203-1714 USA; Michael L. Dent, Anteon Corporation USA; William J. Hardman, Naval Air Systems Command, Propulsion and Power Directorate (AIR 4.4.2), Patuxent River, MD 20670-1534 USA; Paul Hoffman, United States Navy, NAVAIR, Patuxent River, MD 20670 USA; J. Wayne Jones, University of Michigan, College of Engineering, Department of Materials, Science and Engineering, Ann Arbor, MI 48109 USA; Stephan M. Russ, Air Force Research Laboratory, Materials and Manufacturing Directorate, AFRL/MLLN, Wright-Patterson Air Force Base, OH 45433-7817 USA

Wednesday AM — Room: La Galerie 5
September 29, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Michael Caton, Air Force Research Laboratory, Wright-Patterson AFB, OH 45433 USA; Noel E. Ashbaugh, University of Dayton Research Institute, Dayton, OH 45469-0128 USA

8:30 AM Invited
Simulation of Deformation Modes for Damage Detection in Turbine Engine Disks: *Robert Brockman*[1]; Reji John[2]; [1]University of Dayton Research Institute, Dayton, OH 45469-0128 USA; [2]Air Force Research Laboratory, Metals, Ceram., & NDE, 2210 Tenth St., Ste. 1, Bldg. 655, Wright Patterson AFB, OH 45433-7817 USA

Recent studies have shown that analytical predictions of crack growth in rotating components can be used in conjunction with displacement measurement techniques to identify critical levels of fatigue damage. However, investigations of this type traditionally have focused on the detection of damage at known flaw locations. This presentation will address the related problem of assessing damage associated with flaws at unknown locations, through the combined use of analytical models and measured vibration signatures. Because the measured data are insufficient to identify a unique solution for the location and severity of fatigue cracks, the analytical procedure must be able to bound the extent of damage occurring at life-limiting locations. The issue of analyzing successive measurements to improve estimates of worst-case damage and crack locations will also be discussed.

8:55 AM Invited
Behavior of Nonlinear Acoustic Beta Parameter for Fatigue of a Nickel-Base Superaloy: *Noel E. Ashbaugh*[1]; Eric L. Burke[1]; S. Satish[1]; S. L. Freed[1]; [1]University of Dayton Research Institute, 300 College Park, Dayton, OH 45469-0128 USA

Studies of nonlinear acoustic properties in metallic materials show promise as a NDE technique for early detection of fatigue damage. This early damage before identifiable crack initiation or during the formation of microcracks is a significant portion of fatigue life of a component. Quantification of this precursor damage becomes is an important factor in knowing the health of the material and in damage prognosis. The goal of this investigation is to evaluate the efficacy of the beta parameter that is associated with the nonlinear acoustic behavior of a metal. When a wave pulse is introduced in a metal, harmonic frequencies of increasing amplitude can be detected as fatigue damage accumulates. The amplitude generated for the second harmonic frequency is proportional to the beta parameter. The results of the beta parameter evaluation for early detection of fatigue damage in a nickel-base superalloy at elevated temperature will be discussed.

9:20 AM
Microscopic Laser Ultrasonics for Determining Microstructure Changes Due to Material Degradation: *David Howard Hurley*[1]; Ken L. Telschow[1]; Vance A. Deason[1]; [1]Idaho National Engineering and Environmental Laboratory, Physics Grp., PO Box 1625, Idaho Falls, ID 83415-2209 USA

We report on two laser-based ultrasonic studies geared at measuring various components of materials degradation. These studies span the spectrum from fundamental studies involving idealized single component materials to applied studies involving multicomponent multiphase alloys.
In the first portion of this talk, the application of laser-based Resonant Ultrasound Spectroscopy (RUS) to characterize fatigue hardening will be discussed. Results are presented on a WASP alloy before and after work

hardening and clearly show the effects of hardening. While this approach offers a noncontacting, fieldable approach to determination of material degradation, these results are empirical, requiring material dependent calibration. In the second portion of this talk, fundamental work involving imaging of the interaction of surface acoustic waves with individual grain boundaries will be discussed. In addition to exhibiting sensitivity to grain orientation mismatch, our results suggest that careful analysis of the reflected acoustic component can be used to characterize the subsurface grain boundary orientation. This work is helping lead to a fundamental understanding of elastic wave interaction with selective microstructural features that are well known indicators of fatigue damage.

9:45 AM
Tracing the Fatigue Damage Precursor with Laser Scanning Technique (LST): *Vladimir B. Markov*[1]; Benjamin B. Buckner[1]; James C. Earthman[2]; Joel Angeles[2]; [1]MetroLaser, Inc., 2572 White Rd., Irvine, CA 92614 USA; [2]University of California, Dept. of Chem. Engrg. & Matls. Sci., Irvine, CA 92697-2575 USA

Metal components subjected to cyclic stress develop surface-evident defects (microcracks, slipbands, etc). Monitoring the formation and evolution of these fatigue damage precursors (FDPs) with increasing numbers of cycles can be an effective tool for determining the fatigue state of the component, which can be used in remaining fatigue life prognostics. In this report we discuss a laser scanning technique (LST) proposed for FDP detection and present experimental results from examination of specimens made of nickel-based superalloy and aluminum. The proposed detection technique is based on scanning a focused laser beam over the specimen surface and detecting variations in spatial characteristics of the scattered light signal. These variations indicate the presence of surface abnormalities and therefore can be associated with incremental fatigue damage formation. The studies performed show that the proposed LST can serve as a basis for design of a portable non-contact instrument for in situ structural health monitoring.

10:10 AM Break

10:20 AM Invited
Embedded Piezoelectric Wafer Active Sensors for Material Damage Diagnosis and Prognosis: *Victor Giurgiutiu*[1]; [1]University of South Carolina, Dept. of Mechl. Engrg., 300 S. Main St., Columbia, SC 29208 USA

Piezoelectric-wafer active sensors (PWAS) are small, inexpensive, non-invasive, elastic wave generators/receptors that can be permanently affixed to a structure. Thus, they form an embedded active sensors solution that can be effectively used for material damage diagnosis and prognosis. PWAS are wide-band non-resonant devices. They can be wired into sensor arrays and connected to data concentrators and wireless communicators. PWAS have the potential to bring about a revolution in structural health monitoring, damage diagnosis and prognosis, and non-destructive evaluation. However, the development of PWAS transducers is not yet complete, and a number of issues have still to be resolved. The paper will present research the use of PWAS for material damage diagnosis and prognosis for structural health monitoring through: (a) the tuned traveling Lamb waves approach using the pitch-catch and the pulse echo methods, and (b) the broadband standing Lamb wave approach using the high-frequency electromechanical (E/M) impedance method.

10:45 AM Invited
Ultrasonic In-Situ Characterizatin of Material Damage: *T. E. Michaels*[1]; B. Mi[1]; J. E. Michaels[1]; L. J. Jacobs[2]; J. Qu[3]; [1]Georgia Institute of Technology, Electl. & Computer Engrg., Atlanta, GA 30332-0250 USA; [2]Georgia Institute of Technology, G. W. Woodruff Sch. of Mechl. Engrg., Atlanta, GA USA; [3]Georgia Institute of Technology, Civil & Environ. Engrg., Atlanta, GA USA

Integral to a successful structural prognosis system are sensors to accurately determine the current state of material damage. It is important to detect and characterize damage at the earliest possible stage, as well as to accurately track damage progression during the life of the component. Permanently mounted ultrasonic sensors have the potential for detection of damage on multiple scales depending upon the measurement method, sensor locations and sensor characteristics. High frequency ultrasonic waves are sensitive to small flaws in a local area, whereas lower frequency waves can travel long distances and are thus sensitive to larger defects within an enlarged area. The ability to make differential measurements enhances the ability of ultrasonic sensors to detect and characterize damage. It is shown that the same sensors can be used to perform both global and local measurements depending upon the frequency of excitation and the analysis method used. Results are shown for aluminum specimens subjected to low cycle fatigue using both coherent and diffuse ultrasonic methods.

11:10 AM
Utilizing Ultrasonic Fatigue to Study the Effect of Microstructure on the Fatigue Life of a Titanium Alloy: *Christopher J. Szczepanski*[1]; A. Shyam[1]; S. K. Jha[2]; J. M. Larsen[3]; C. J. Torbet[1]; J. W. Jones[1]; [1]University of Michigan, Dept. of Matls. Sci. & Engrg., HH Dow Bldg., 2300 Hayward, Ann Arbor, MI 48109-2136 USA; [2]Universal Technology Corporation, Dayton, OH 45432 USA; [3]Air Force Research Laboratory, Matls. & Mfg. Direct., AFRL/MLLMN Wright Patterson AFB, Dayton, OH 45432 USA

The effect of microstructural variability on the fatigue life of the near alpha, alpha + beta titanium alloy, Ti-6246, has been examined in the very long life fatigue regime using ultrasonic fatigue. Tests were conducted at ambient temperatures at a frequency of 20 kHz and a load ratio of 0.05. Fatigue lifetimes were characterized in the regime from 106 to 109 cycles. Microstructural features associated with crack initiation and their locations relative to the specimen surface are examined and compared to the behavior observed in conventional fatigue tests. The growth of small cracks during fatigue was examined by measuring the growth of cracks initiating from micronotches produced by femtosecond pulsed laser machining. The fatigue life in Ti-6246 is modeled from the initiation and propagation behavior of the alloy.

11:35 AM
Nondestructive Characterization of Thermal Aging Effects on Mechanical and Fracture Properties of 1Cr1Mo0.25V Steel Using Ball Indentation: Chang-Sung Seok[1]; Jeong-Pyo Kim[1]; E. S. Park[1]; *K. L. Murty*[2]; [1]Sungkyunkwan University, Sch. of Mechl. Engrg., 300 Chunchun-dong, Jangan-gu, Suwon, Kyonggi-do 440-746 Korea; [2]North Carolina State University, Nucl. Engrg., 2800 Stinson Dr., PO Box 7909, Raleigh, NC 27695-7909 USA

Effect of thermal aging on mechanical and fracture characteristics of 1Cr-1Mo-0.25V steel was investigated following heat treatment at 630C (903K) for varied times up to 1820 hours (~75 days). Tensile and fracture (K_{1C}) tests were performed at room temperature before and following thermal aging that indicated decreased strength and fracture toughness (K_Q) with corresponding increase in ductility. Microstructure of the aged material revealed coarsening of carbides and precipitates. Ball indentation (BI) technique used as a nondestructive tool to characterize the aging effects, involved multiple loading-unloading cycles from which true stress versus strain data could be obtained. In addition, an estimation of the fracture toughness could also be made based on indentation energy to fracture (ICF). These data are also compared with those obtained from electrical resistivity and ultrasonic attenuation. A major advantage the technique is the application to small specimens in essentially nondestructive fashion with the possibility for field application for on-line condition monitoring of the structures.

Materials Damage Prognosis: Local and Global Methods and Sensors for Interrogation of Materials Damage State II

Sponsored by: TMS - Structural Materials Division
Program Organizers: James M. Larsen, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson AFB, OH 45433-7817 USA; Jeffrey R. Calcaterra, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson Air Force Base, OH 45433-7817 USA; Leo Christodoulou, Defense Advanced Research Agency, Arlington, VA 22203-1714 USA; Michael L. Dent, Anteon Corporation USA; William J. Hardman, Naval Air Systems Command, Propulsion and Power Directorate (AIR 4.4.2), Patuxent River, MD 20670-1534 USA; Paul Hoffman, United States Navy, NAVAIR, Patuxent River, MD 20670 USA; J. Wayne Jones, University of Michigan, College of Engineering, Department of Materials, Science and Engineering, Ann Arbor, MI 48109 USA; Stephan M. Russ, Air Force Research Laboratory, Materials and Manufacturing Directorate, AFRL/MLLN, Wright-Patterson Air Force Base, OH 45433-7817 USA

Wednesday AM Room: La Galerie 6
September 29, 2004 Location: Marriott New Orleans Hotel

Session Chairs: Paul Hoffman, United States Navy, NAVAIR Struct. Div., Patuxent River, MD 20670-1906 USA; John Papazian, Northrop Grumman, Airborne Early Warning & Elect. Warfare, Bethpage, NY 11714 USA

8:30 AM Invited
Demonstration of Advanced Prognostic Health Management Approach for Gas Turbine Engine Disks: *Jerrol Littles*[1]; Bradford A. Cowles[1]; Richard A. Holmes[1]; Richard G. Pettit[1]; John J. Schirra[1]; Stephan M. Russ[2]; Andrew H. Rosenberger[2]; James M. Larsen[2]; [1]Pratt & Whitney, 400 Main St., E. Hartford, CT 06108 USA; [2]Air Force Research Laboratory, 2230 Tenth St., Ste. 1, Wright-Patterson AFB, OH 45433 USA

As part of the DARPA-funded Materials Prognosis program, Pratt & Whitney conducted two spin tests of IN100 minidisks. The objective of the tests was to demonstrate the benefits of advanced fatigue crack growth predictive tools under dwell fatigue conditions, as well as to demonstrate the ability to infer component damage state from in-situ sensed component response. These tests demonstrated a significant advance toward developing an approach for performing real-time prognostic health management assessments. Both 3D fracture mechanics tools and the state-awareness sensing proved key to the over-all success of these tests.

8:55 AM Invited

Successes and Failures for LCF Rotor Burst Prognosis Using Blade-Tip Sensors: *Andreas Von Flotow*[1]; Peter Tappert[1]; Mathieu Mercadal[1]; William Hardman[2]; [1]Hood Technology Corporation, Hood River, OR 97031 USA; [2]NAWCAD

Turbomachinery rotors deform due to centripetal loads. The deformation is a function of rotational speed. As a flaw develops in the rotor, this deformation changes. This changing deformation can identify the underlying flaw. A practical way to measure shape of a spinning rotor is with sensors at the rotor blade tips. This paper describes successes and failures in efforts to anticipate rotor burst with blade tip sensors. Several successes are described, as well as several failures.

9:20 AM

Spin Pit Crack Growth Evaluation of Materials-Based Prognosis Concept: *Jeffrey L. Williams*[1]; Robert H. VanStone[1]; Bernard H. Lawless[1]; Dennis M. Corbly[1]; Genghis Khan[2]; Ahmet Kaya[2]; [1]GE Transportation - GE Aircraft Engines, 1 Neumann Way, Cincinnati, OH 45215 USA; [2]GE Global Research, Niskayuna, NY 12301 USA

The feasibility of a materials-based prognosis concept was evaluated through spin pit crack growth testing of full-scale military turbine engine disks. Efforts included detailed stress analysis, analytical crack growth predictions, and assessment of crack detection sensors. Comparison of laboratory crack growth specimens and spin-pit pit hardware were conducted to assess differences between specimens and field hardware and the influence of test environment. Quantitative fractography was performed to define crack dimensions for specific cycle counts and to evaluate 3D-FEM crack growth analyses. The environment of the spin pit chamber, geometry of the cracks, and the manufacturing-induced residual stress in the disk were determined to have significant effects on the test results. The present paper will focus on the fractographic findings of a test article with four growing cracks, one of which propagated to catastrophic failure. These results lend insight to the complex range of material state variables that must be accounted for to implement a prognosis system for turbine disks.

9:45 AM Invited

Integrated Engine Prognostics and Health Management (IEPHM) System: *Kiyoung Chung*[1]; [1]GE Aircraft Engines, 1-Neumann Way, BBC-5, Cincinnati, OH 45215 USA

This paper describes the results of a NAVAIR sponsored DUST program that developed and demonstrated a diagnostic/prognostic system for aircraft engines. The specific objectives of the program are: 1) to develop highly modular system architecture for the aircraft engine PHM system that can be easily scaled, 2) to demonstrate the system flexibility in accommodating various, dissimilar diagnostic/prognostic modules and 3) to conduct on-engine demonstration of the system. The IEPHM architecture integrates a high fidelity, real-time engine model, model-based functions such as diagnostic/prognostic algorithms and on-line life usage tracking, and sensor-based functions such as vibration analysis and inlet/exhaust debris monitoring. The IEPHM system also integrates all existing FADEC (Full Authority Digital Engine Control) diagnostic status as evidentially information into the decision making tool called, Gas-Path Reasoner. This information fusion tool employs a multi-layered architecture to yield robust, accurate real-time PHM outputs. This paper also presents results from system bench testing as well as those from an engine test conducted to validate and mature the integrated engine prognosis system architecture.

10:10 AM Break

10:20 AM

Arrayed Multiple Sensor Networks for Material and Structural Prognostics: *Trevor Niblock*[1]; Harshal Surangalikar[1]; Jose Moreno[1]; [1]Analatom Incorporated, 562 Weddell Dr., Ste. 4, Sunnyvale, CA 94089-2108 USA

In this paper a lightweight, low cost sensor array system capable of monitoring numerous physical phenomena is described. The system is designed to incorporate modern manufacturing attributes (e.g. quality) with the latest MEMS (Micro Electro Mechanical Systems) technology to produce robust systems that are both low cost and meet all functionality requirement of a fully integrated prognostics system. The system is designed to act as a portal sensor(s) and a central data repository. Key features of the system are; multiple sensor interfacing, low power, low cost, multiple portal interface (e.g. BUS) and adaptability onto numerous networks. Local processing is at a variable rate that is self-determined. This algorithm is based on conditioning that can be updated by a larger prognostic system further up the logic chain. The system also analyses individual sensor output and parallel sensor output to look for trends and inconsistency.

10:45 AM

Identification of Propagating Elastic Waves and Incipient Damage in a Friction Stir Welded Al-Li Plate for Cryogenic Tank Applications: *Shankar Sundararaman*[1]; Muhammad Haroon[1]; Douglas Adams[1]; Kumar V. Jata[2]; [1]Purdue University, Sch. of Mechl. Engrg., Rey Herrick Labs., 140 S Intramural Dr., W. Lafayette, IN 47907 USA; [2]Air Force Research Laboratory, Metals, Ceram., & NDE Div., 2230 Tenth St., WPAFB, OH 45433 USA

Organic matrix composite as well as Al-Li metal tanks are being considered by the United States Air Force for the next generation space launch and space operations vehicles. Al-Li alloys can offer substantial weight reduction with reduced susceptibility to leakage. Unlike in expendable tanks, reusability and quick turnaround time between missions are key considerations for future space launch and operations. Therefore, identification, quantification and location of damage on the reusable cryotanks have become key drivers in achieving the safety and life-cycle cost objectives of the Advanced Space Transportation Program. This work investigates acoustic impedance and wave propagation sensing and data interrogation methodologies for extracting features that can potentially be used to identify incipient damage in the form of gradients in dislocation densities in a friction stir Al-Li butt weld. Wave propagation characteristics are first examined in the Al-Li plate, friction stir welded heat affected zone and across this zone to identify discontinuities and baseline reflection patterns due to boundaries and scalloped weld patterns. Localized temperature gradients are then used to simulate local changes in weld material density in static tests to mimic dislocation density gradients along the weld and elastic waves are propagated through the weld to detect these incipient forms of damage. It is demonstrated that such techniques could potentially be used to assist in quick offline inspection of cryogenic tank material systems.

11:10 AM

Development of Automated Damage Detection Techniques: *Mark M. Derriso*[1]; [1]Air Force Research Laboratory, VASA, 2790 D. St., Wright Patterson AFB, OH 45433 USA

To meet turn-around goals of future Air Force launch vehicles, the time required to assess the structural condition after a mission needs to be significantly reduced. Specifically, an automated system is needed which can assess the health of the entire structure within hours of the completed mission and re-certify the structure for flight. Structural health monitoring (SHM) refers to automated methods for determining degradation in the integrity of mechanical systems. Damage may include loose or missing fasteners, cracks, delaminations, or impact damage. The thermal protection system (TPS) is a critical component of space vehicles. Although actual thermal protection systems (TPS) will likely be constructed of composite materials and/or high temperature metal alloys, an aluminum plate demonstration article is used to represent a TPS element for laboratory testing. Damage resulting due to loose or missing fasteners and cracking can be simulated with the aluminum plate article. A combined analytical and experimental approach is being utilized to develop SHM techniques capable of detecting, locating, and assessing damage. Vibration-based techniques are used for the studies on loose or missing fasteners. The aluminum plate is excited using a piezoelectric transducer with additional piezoelectric sensors use to detect the response. Features extracted from the measured data are input to a statistical pattern classifier to locate and quantify the fastener damage. Finite element analyses are used to provide a physics-based understanding of the extracted features. Preliminary results from aluminum plate studies with loose or missing fasteners show that the SHM system is extremely accurate at detecting and locating missing fasteners, but less accurate at detecting, locating, and assessing loose fasteners. The modal methods used for the fastener studies are not suitable for detecting cracks; therefore, ultrasonic wave techniques are under consideration for the crack studies. For these studies, piezoelectric transducers will be used to create and measure guided waves in the plate. As with the fastener studies, features extracted from the measured data will be input to a statistical pattern classifier to locate and quantify material cracking. The crack studies will benefit from the maturity of the pattern recognition platform previously developed.

11:35 AM

Physically-Based Health Management Tool for Improved Prognostics and Diagnostics of Turbine Engines: *Doug W. Akers*[1]; [1]Positron Systems, Inc., 6151 N. Discovery Way, Boise, ID 83713 USA

Thermomechanical (TMF) damage in turbine engine components results in excessive maintenance costs, reduction of operational readiness, and is a leading cause of engine failures. Significant improvements have been made in nondestructive inspection technologies to resolve several difficult fatigue-related turbine engine problems, however, there remain significant challenges to reduce TMF related engine failures, improve fleet readiness and significantly reduce maintenance costs. A reliable inspection tool has been developed to provide an integrated measurement/modeling technology that can be used to nondestructively assess the effects of TMF and foreign object damage in turbine engine components, along with assessing the beneficial effects of surface treatment enhancements. Distributed Source Positron Annihilation measurement technology evaluates operational damage and induced residual stress effects based upon measuring changes in the defect density and chemical changes induced in the material. Recent developments allow for in-situ inspection of aircraft turbine engine components without disassembly of the engine for examination.

Mechanical Behavior of Body-Centered-Cubic (BCC) Metals and Alloys: Yielding and Plastic Flow

Sponsored by: TMS - Structural Materials Division, TMS - SMD-Mechanical Behavior of Materials-(Jt. ASM-MSCTS), TMS - SMD-Refractory Metals Committee, TMS - SMD-Structural Materials Committee

Program Organizers: George T. Gray III, Los Alamos National Laboratory, Dynamic Properties Team, Los Alamos, NM 87545-0001 USA; Thomas R. Bieler, Michigan State University, Department of Chemical Engineering and Materials Science, East Lansing, MI 48824-1226 USA; John J. Lewandowski, Case Western Reserve University, Department of Materials Science and Engineering, Cleveland, OH 44106 USA; Eric M. Taleff, University of Texas, Mechanical Engineering Department, Austin, TX 78712-1063 USA

Wednesday AM — Room: Mardi Gras Ballroom A
September 29, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: John J. Lewandowski, Case Western Reserve University, Dept. Metall. & Matls. Sci., Cleveland, OH 44106 USA; Eric M. Taleff, University of Texas, Mechl. Engrg., Austin, TX 78712-0292 USA

8:30 AM
Yield Stress Prediction for Second Period BCC Alloys at Ambient Temperature: *David L. Davidson*[1]; [1]Southwest Research Institute (Retired), 117 Elm Spring, San Antonio, TX 78231 USA

Analysis of existing test data for Nb-Mo and Mo-Re alloy single crystals (high purity materials) has resulted in development of a semiempirical method for predicting the yield stress of single phase alloys based on these elements. Part of the process required computation of the magnitude of the Peierls-Nabarro stress from elastic constants and lattice parameter. It was also necessary to derive a yield stress for polycrystalline alloys from the single crystal results. The prediction process was tested against several Nb-Cr-Ti alloys, which validated the method.

8:50 AM
Solid-Solution Softening in BCC Mo by First Principles: *Dallas R. Trinkle*[1]; Christopher F. Woodward[1]; Satish Rao[1]; [1]Air Force Research Laboratory, Wright Patterson AFB, OH 45433-7817 USA

Solid solution softening observed in the group VA and group VIA transition metals has traditionally been attributed to either extrinsic—such as interstitial scavanging—or intrinsic—direct solute/dislocation interaction—effects. We have applied different first principles methods—ultrasoft pseudopotentials, PAW, and LAPW—to evaluate possible intrinsic solid-solution-softening in the group VI BCC transition metals. First, we calculated the size and modulus misfit parameters of solid solutions in Mo as suggested by the work of Fleischer. Second, we calculated the change in the primary Peierls barrier when Re, Hf, and W solutes are introduced along a straight a/2<111> screw dislocation in Mo. Here the local strain field associated with the dislocation core is self-consistently coupled to the long-range elastic field using the recently developed lattice Greens Function Boundary Condition method. Results from these two methods will be contrasted and compared to available experimental results.

9:10 AM
Strain Hardening Prediction for Second Period BCC Metals and Alloys: *David L. Davidson*[1]; [1]Southwest Research Institute (Retired), 117 Elm Spring, San Antonio, TX 78231 USA

The basis for this analysis was TEM observations of dislocation structures below the transition temperature. A review of the models for strain hardening that are compatible with TEM results revealed that Mughrabi's models (there are 4) were the most applicable. Analysis of published stress-strain curves for Nb-Mo and Mo-Re single crystals (high purity) were used to derive model parameters, and it was found that the magnitude of some of parameters were alloy insensitive, but others were dependent on composition, but with no predictable trends (to date). Thus, it appears as though the ability to predict the strain hardening behavior of transition metal alloys is limited until a better understanding of compositional parametric trends or more complex models become available.

9:30 AM
Grain Size and Hardness Variation in Vapor Deposited BCC Metals: *Alan F. Jankowski*[1]; [1]Lawrence Livermore National Laboratory, Chmst. & Matls. Sci., PO Box 8080, MS L-352, Livermore, CA 94551-9900 USA

Vapor deposition methods are used to prepare fully dense foils of the bcc metals, vanadium and tantalum. Electron-beam evaporation is the method used to prepare foils with grain sizes that range from the micron-to-millimeter scale. Single crystals have been produced that are tens of microns thick with lateral dimensions in excess of several millimeters square. Magnetron sputter deposition is the method used to prepare foils with grain sizes that range from the micron-to-nanometer scale. Preliminary micro-hardness measurements of large grain deposits are in agreement with reference values of 1.4 GPa or less for vacuum annealed specimens of each metal. For specimens with micron-scale grain size, a significant increase is measured in the micro-hardness. The micro-hardness of vanadium increases to 2.7 GPa and for tantalum to 2.9 GPa. The characterization of the microstructure in these vapor deposits will be presented using Bragg and Laue x-ray diffraction, as well as scanning and transmission electron microscopy. This work was performed under the auspices of the United States Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

9:50 AM Break

10:10 AM
Tensile and Long-Time Creep Behavior of Nb-1%Zr-0.1%C Sheet as Affected by Thermomechanical Processing: *Mehmet Uz*[1]; Robert H. Titran[2]; [1]Lafayette College, Chem. Engrg. Dept., 262 AEC, Easton, PA 18042 USA; [2]NASA-GRC (Retired), 15976 Walnut Creek Dr., Strongsville, OH 44149 USA

Effects of thermomechanical processing on the tensile and creep properties of Nb - 1 wt.%Zr - 0.1 wt.%C, a candidate alloy for use in advanced power systems, were studied. Sheet bars were cold rolled into 1-mm thick sheets following single, double, or triple extrusion operations at 1900 K. All the creep and tensile specimens were given a two-step heat treatment that consisted of 1 h at 1755 K and 2 h at 1475 K prior to testing. Creep tests were conducted at 1350 K and 34.5 MPa for times ranging from about 10,000 to 19,000 h, and at 1450 K and 24 MPa for up to 12,000 h. Tensile properties were determined at both 300 K and 1350 K. The results are discussed in correlation with the thermomechanical processing and the resulting microstructure, and they are also compared to results obtained from the testing of Nb - 1 wt.%Zr and Nb - 1 wt.%Zr - 0.06 wt.%C alloys. This work was performed for USDOE, Nuclear Energy, Reactor Sys. Development and Tech., Washington, D.C. 20545, under Interagency Agreement DE-AI03-86SF16310.

10:30 AM
Tensile and Thermal Creep Behavior of V-4Cr-4Ti: *Meimei Li*[1]; David T. Hoelzer[1]; Martin L. Grossbeck[1]; Scott E. O'Rourke[2]; [1]Oak Ridge National Laboratory, Metals & Ceram., PO Box 2008, MS-6138, Oak Ridge, TN 37831-6138 USA; [2]University of Tennessee, Dept. of Nucl. Engrg., Knoxville, TN 37996 USA

The objective of this study is to evaluate and understand the influence of environment on the mechanical behavior of the solid solution V-4%Cr-4%Ti alloy by exposure to liquid lithium. This alloy is a candidate for structural applications in fusion systems, particularly attractive for a liquid lithium coolant/breeder blanket system. Tensile property measurements over a wide range of strain rates and temperatures and thermal creep measurements between 650 and 800°C in vacuum environments have shown that interstitial impurity elements such as oxygen, carbon, and nitrogen can significantly affect the mechanical properties of the alloy. Effects include an increase in yield strength, loss of tensile ductility, and reduced low temperature fracture toughness. The magnitude of the effects is strongly dependent upon the distribution of the impurity elements in the microstructure. In fact, interstitial impurities can have a beneficial effect on high temperature creep. Rupture times were found to be shorter and the creep strain rates higher in highly-purified V-4Cr-4Ti compared to the original heat. Preliminary studies of the thermal creep of V-4Cr-4Ti in liquid lithium revealed that the creep strain rate was higher than in vacuum due to loss of oxygen during exposure to lithium. Since a liquid lithium environment can change the concentration of interstitial impurities in the alloy, the effect on mechanical properties must be determined. The tensile properties and thermal creep behavior of V-4Cr-4Ti are being examined for liquid lithium exposure at 700 and 800°C up to 2000 h. Under these conditions, oxygen is removed from vanadium alloys, and carbon and nitrogen can be transferred to vanadium alloys from liquid lithium. The paper will present experimental results on tensile properties of V-4Cr-4Ti after lithium exposure and creep behavior during lithium exposure, and compare with results obtained in vacuum environments. The paper will address the effect of oxygen on tensile strength and high temperature creep strength, and correlate microstructural development with static and time-dependent plastic properties.

10:50 AM
Abnormal Dynamic Grain Growth During Creep Deformation in Commercial-Purity, Power-Metallurgy (PM) Grade Mo Sheet: *James R. Ciulik*[1]; Eric M. Taleff[1]; [1]University of Texas, Matls. Sci. & Engrg., 160 E. Dean Keaton St., ETC 9.170, Austin, TX 78705 USA

Commercial-purity, powder-metallurgy grade Mo sheet was subjected to tensile testing at slow strain rates, less than 10-4 s-1, and temperatures from 1300°C to 1700°C. At 1500°C and above, abnormal dynamic grain growth resulted after accumulation of a critical strain. Prior to deformation, the sheet was recrystallized (20 to 70 um diameter grains). Under conditions which initiated abnormal dynamic grain growth, the recrystallized grain structure abruptly transformed to a structure consisting of grains several millimeters in diameter, resulting in a dramatic decrease in creep strength. This behavior is compared to that of the same material tested at 1400°C, for which abnormal grain growth did not occur. Creep tests were performed under two conditions: constant-temperature strain-rate-change (SRC) tests over rates from 1.0*10-6 to 5.0*10-4 s-1, and constant-temperature elongation-to-failure (EF) tests within this range. Data from these tests are used to characterize abnormal dynamic grain growth and its effect on creep deformation behavior.

11:10 AM
Elevated Temperature Strength of Cr-W Alloys: *Omer N. Dogan*[1]; Karol K. Schrems[1]; [1]U.S. Department of Energy, Albany Rsch. Ctr., 1450 Queen Ave., SW, Albany, OR 97321 USA

Cr alloys containing 0-30 weight percent W were investigated for their strength and ductility. These experimental alloys are intended for use in elevated temperature applications. Alloys were melted in a water-cooled, copper-hearth arc furnace. Microstructure of the alloys was studied using X-ray diffraction, scanning electron microscopy, and light microscopy. A hot hardness tester was used to study the strength of these materials up to 1200ºC. Compression tests at the same temperature range were also conducted.

11:30 AM
Role of Laves Phases on the Mechanical Properties of Multicomponent Nb-Ti-Si-Cr-Al-X Alloys: *Raghvendra Tewari*[1]; Hyojin Song[1]; Vijay K. Vasudevan[1]; Amit Chaterjee[2]; [1]University of Cincinnati, Dept. of Chem. & Matls. Engrg., Cincinnati, OH 45221 USA; [2]Rolls Royce Corporation, Indianapolis, IN 46206 USA

Of late, Nb-Ti-Cr-Si-Al-X alloys have been considered as candidate materials for high-temperature structural applications in aero engines. Using a multicomponent approach, attempts are being made to obtain good strength with adequate oxidation resistance at operating temperatures (~800-1000°C) in these alloys. In the microstructure of the Nb-Ti-Cr-Si based alloys, which essentially consist of the silicide phase and the bcc β matrix, the presence or absence of the Laves phase can bring about considerable changes in the mechanical properties. The present paper focuses on the formation of the Laves phase in the β matrix. Different morphologies of this phase have been obtained by aging at different temperatures for various durations and the structure, chemistry and volume fraction of these phases has been determined. The crystallographic and kinetic aspects associated with the formation of the Laves phase have been studied. The effect of these phases on the mechanical properties of the alloy system has also been examined.

Modeling and Computer Applications in Metal Casting, Shaping & Forming Processes: Modeling and Computer Applications: Shaping and Rolling Processes

Sponsored by: AIST, TMS - Extraction & Processing Division, TMS - Materials Processing & Manufacturing Division, TMS, TMS - MPMD/EPD-Process Modeling Analysis & Control Committee, TMS - MPMD-Shaping and Forming Committee, TMS - MPMD-Solidification Committee, AIST - Division VI, AIST - Division VII, TMS - MPMD-Computational Materials Science & Engineering-(Jt. ASM-MSCTS)
Program Organizers: Krich Sawamiphakdi, The Timken Company, R&D Manufacturing Technology, Canton, OH 44706 USA; Praveen Pauskar, The Timken Company, Advanced Process Technology, Timken Research, Canton, OH USA; Maciej Pietrzyk, Akademia Gorniczo-Hutnicza, Department of Computer Methods in Metallurgy, Krakow Poland; Raghavan Srinivasan, Wright State University, Department of Mechanical & Materials Engineering, Dayton, OH 45435 USA; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA; Brian G. Thomas, University of Illinois, Department of Mechanical and Industrial Engineering, Urbana, IL 61801 USA

Wednesday AM — Room: La Galerie 2
September 29, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Maciej Pietrzyk, University of Science and Technology, Krakow 30-059 Poland; Raghuvan Srinivasan, Wright State University, Mechl. & Matls. Engrg. Dept., Dayton, OH 45435 USA

8:30 AM
A New Steady-State FE Process Model for the Prediction of Plastic Deformation in Shape Rolling of Complex-Shaped Products: *Sang Moo Hwang*[1]; [1]Pohang University of Science and Technology (POSTECH), Dept. of Mechl. Engrg., Pohang, 790-784 Korea

A new, finite element-based, steady-state process model is presented for the prediction of plastic deformation in shape rolling. Described are a full, three-dimensional finite element model for the analysis of plastic deformation, a new streamline tracing scheme, and the schemes for predicting the free surface, including the contact area between the roll and workpiece. The model's prediction accuracy is examined through comparison with measurements. The model is then applied to multi-pass rolling of a variety of commercial products, with emphasis on demonstrating the model's capability to deal with rolling with complex-shaped products.

8:55 AM
Prediction of Strip Profile in Four-High Mills by the Finite Element Method: *Sang Moo Hwang*[1]; [1]Pohang University of Science and Technology (POSTECH), Dept. of Mechl. Engrg., Pohang, 790-784 Korea

In hot and cold strip rolling, a capability for precisely predicting the strip profile is extremely important in process control to obtain products with the desired product dimensions. In this paper, we present a full, finite element-based approach for the precision analysis of the strip profile in four high mills. Described are basic finite element models for the analysis of strip deformation, work roll deformation, and backup roll deformation. Also described is an iterative strategy for the treatment of mechanical contact at the work roll-strip interface as well as at the work roll-backup roll interface. A series of process simulation are conducted to examine the validity of the proposed approach through comparison with the measurements. Also examined is the prediction accuracy of the existing on-line model through comparison with the predictions from the proposed approach.

9:20 AM
Process Simulation for Industrial Rolling Applications: *Dave Lambert*[1]; [1]Scientific Forming Technologies Corporation, 5038 Reed Rd., Columbus, OH 43220 USA

DEFORM is a well-known Finite Element Analysis system used for metal forming process simulation. Recent developments include the ability to model multiple deforming body behavior during multi-pass pack rolling and microstructure prediction during multi-pass shape rolling. Preliminary work on ring rolling simulation is also reported. The current work details how DEFORM can be applied to a number of rolling processes and describes latest developments carried out on a rolling template.

9:45 AM
Finite Element Model for Efficient Simulation of Ring Rolling: Zbigniew Malinowski[1]; Miroslaw Glowacki[2]; *Maciej Pietrzyk*[3]; Wieslaw Madej[4]; [1]University of Science and Technology, Heat Engrg. & Environ. Protection, Mickiewicza 30, Krakow 30-059 Poland; [2]University of Science and Tech-

nology, Computer Sci. in Industry, Mickiewicza 30, Krakow 30-059 Poland; [3]University of Science and Technology, Computer Methods in Metall., Mickiewicza 30, Krakow 30-059 Poland; [4]University of Science and Technology, Metal Forming, Mickiewicza 30, Krakow 30-059 Poland

Ring rolling is one of the most difficult metal forming processes for the finite element simulation. Deformation of the material is imposed in a large number of passes, often exceeding hundred. These passes are performed in the two pairs of rolls usually with complex shapes. Moreover, the gap between the rolls is changing continuously what means that each point on the circumference of the ring is subjected to slightly different deformation history. Several examples of the finite element analysis of this process can be found in the literature, see for example,[1-2] but the solutions are usually constrained to one pass. Extending these simulations to large number of passes will involve so large computing times that application of the model in the industrial practice will not be possible. Authors of this paper propose a new approach to this problem. This approach is based on the fully three-dimensional solution, which, however, is performed for some average rolling parameters during one rotation of the ring. The details of the model and the boundary conditions are presented in the paper and a set of results obtained for a selected ring rolling process is demonstrated. The computing times, which are still very long, are much shorter comparing to use of fully dimensional model to subsequent passes. Application of the proposed finite element program to simulation of the real technological process and to aiding of the ring rolling technology design is shown in the paper. [1]Z.J. Szabo, E. Dittrich, Manufacturing System for the Production of Seamless-Rolled Rings, Mat. 6 Konf. Metal Forming'96, eds, Pietrzyk M., Kusiak J., Hartley P., Pillinger I., J. Mat. Proc. Techn., t. 80-81, 1996, 67-72. [2]Z.M. Hu, I. Pillinger, P. Hartley, S. McKenzie, P.J. Spence, Thermo-Plastic Finite-Element Modelling of a Hot Titanium Ring, Mat. Konf. Numiform'95, ed., S.F. Shen, P.R. Dawson, Ithaca, 1995, 941-946.

10:10 AM Break

10:20 AM
Sensitivity of Parameters of Backward-Forward Extrusion Test on Material Properties and Friction: *Maciej Pietrzyk*[1]; Andrzej Zmudzki[1]; Danuta Szeliga[1]; Marcin Papaj[2]; Roman Kuziak[3]; [1]University of Science and Technology, Computer Methods in Metall., Mickiewicza 30, Krakow 30-059 Poland; [2]Non-Ferrous Metal Foundry, Starachowice Poland; [3]Institute for Ferrous Metallurgy, K. Miarki 12, Gliwice 44-100 Poland

The reliable material and friction models are necessary for the accurate computer simulation of the deformation processes. Evaluation of flow stress of materials undergoing the deformation is the prime objective of the plastometric tests, such as tension, torsion and compression. It should be emphasized, however, that each of these tests have several disadvantages. Effect of friction and resulting inhomogeneities of flow are the main disadvantages of compression tests, which are commonly used to determine material properties for bulk forming processes. The friction coefficient has to be known to determine properly the flow stress on the basis of measurements of loads. Thus, simultaneous evaluation of friction and rheological parameters on the basis of one type of the tests was proposed by a number of scientists, see for example.[1] Ring compression is usually selected to perform this analysis. This test shows reasonably high sensitivity on friction, but maintaining the conditions comparable to real processes is always questionable. Therefore, the general objective of the present work is investigation of a new test for evaluation of both material properties of metal alloys and friction parameters. The test, which is based on combine forward-backward extrusion, involves high contact pressure characteristic for metal forming processes. The work is a continuation of Authors' earlier research on the design of the optimal shape of a tool for this test.[2] The particular objective of this work is the finite element simulation of the forward-backward extrusion test and analysis of sensitivity of the measured loads and shape of the extrudate on rheological and friction parameters. Experiments of hot extrusion of aluminum were performed and inverse analysis, which combines FEM simulation with optimization techniques, was applied to determine the investigated parameters. The results are compared with those obtained for the ring compression. [1]Szeliga D., Pietrzyk M., Identification of Rheological and Tribological Parameters, Metal Forming Science and Practice, A State-of-the-art Volume in Honour of Professor J.A. Schey's 80th Birthday, ed., Lenard J.G., Elsevier, Amsterdam, 2002, 227-258. [2]Zmudzki A., Papaj M., Kuziak R., Kusiak J., Pietrzyk M., Optimum Die Shape Design for Evaluation of Material Properties, Proc. ESAFORM 6 Conf., ed., Brucato V., Salerno, 2003, 139-142. [3]Zmudzki A., Gawad J., Kusiak J., Pietrzyk M., Application of Sensitivity Analysis to Die Shape Design for Inverse Analysis of Two-Phase Materials. Proc. COMPLAS VII Conf., Barcelona, 2003, CD-ROM.

10:45 AM
Development and Optimization of the Models for 2050 Hot Rolling Mill Baosteel: *Xuyi Shan*[1]; [1]Baosteel, Hot Rolling Mill Plant, Shanghai 200941 China

Accurate models are the key to the stable rolling and product quality of hot rolling mill production. In the process computer system revamping project of 2050 hot rolling mill of Baosteel, the development and optimization of the models for roughing mill, finishing mill, profile and flatness control and laminar cooling systems are carried out by Baosteel. With a thorough understanding of the structure and a detailed evaluation of the models, the major problems are pinpointed. By developing new models and optimizing the model parameters systematically, the critical problems troubling the production of 2050 hot rolling mill are solved, and the smooth and efficient production of the mill is ensured. At the same time, the product quality is improved dramatically. In this paper, the major problems related to the roughing mill, finishing mill, profile and flatness control and laminar cooling systems are introduced, followed by a brief description of the works carried out in each system, and finally the main improvements are presented.

11:10 AM
Design of Optimal Rolling Schedule Assuring Designed Final Microstructure: *Dmitry S. Svyetlichnyy*[1]; [1]Czestochowa University of Technology, Faculty of Process & Matls. Engrg. & Applied Physics, Al. Armii Krajowej 19, Czestochowa 42-200 Poland

The paper deals with methods of optimal control, which back up evaluation of the thermomechanical flat rolling process. As an example it is considered the strip rolling in the reverse rolling mill. Optimal parameters are defined from the desired final grain size. The austenite and ferrite grain size could be the criterion of optimization. In the paper an algorithm based on the optimal control theory is presented. A state-space model with physical constraints is described. The model consists of the descriptions of the rolling process, recrystallization and grain growth. The optimal discrete trajectories for such control parameters as the final temperature, reductions and interpass time are calculated. The rolling constrains are applied to the control trajectories (reduction, interpass time) and to state-space trajectories (temperature, rolling force and moment). The results of calculations allow for the design of the optimal rolling schedule. In the paper examples of the optimal schedule calculations is presented.

11:35 AM
Simulation of the Rolling Process of 4-High Hot Steel Strip Continuous Mills: *Yingrui Wang*[1]; Zhenshan Cui[1]; Hongmin Liu[2]; [1]Shanghai Jiao Tong University, Dept. of Plasticity Tech., Baolin 3-40-504, Baoshan Dist., Shanghai 201900 China; [2]Yanshan University, Sch. of Mechl. Engrg., Qinhuandao China

The three-dimensional plastic deformations of strip are analyzed by using the stream surface strip element method, the elastic deformations of rolls are analyzed by using the influence coefficient method, the analyzing and computing model of shape and crown is established by combining them, and the rolling process of 1660 mm 4-high hot steel strip continuous mills is simulated. The simulated results tally well with the experimental results. The model and the method for simulation of shape analysis and control of 4-high hot steel strip continuous mills are provided.

12:00 PM
The Effect of Sample Shape on ECAP by Simulation: *Ren Yuan*[1]; T. David Burleigh[1]; [1]New Mexico Institute of Mining and Technology, Dept. of Matls. & Metallurgl. Engrg., 801 Leroy Place Rd., Socorro, NM 87801 USA

In this study, a commercial two-dimensional rigid-plastic model (DEFORM2D) was used to simulate ECAP process of CP titanium with different front shapes of the sample. The results indicate that the sample with a semi-round front was most advantageous to obtain a high and uniform maximum effective strain without a high ram pressure. Comparing the simulated curve of load versus ram displacement, we found the time to reach the maximum load varies with the different front sample shapes. The front shape of the sample contributes to the results of ECAP.

Pb-Free and Pb-Bearing Solders: Session V

Sponsored by: TMS - Electronic, Magnetic & Photonic Materials Division, TMS - EMPMD-Electronic Packaging and Interconnection Materials Committee
Program Organizers: C. Robert Kao, National Central University, Department of Chemical and Materials Engineering, Chungli City 32054 Taiwan; W. Plumbridge, Open University, School of Engineering Materials, Milton Keynes MK7 6AA UK; K. N. Subramanian, Michigan State University, Chemical Engineering & Material Science, East Lansing, MI 48824 USA

Wednesday AM — Room: Grand Ballroom K
September 29, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Elizabeth A. Holm, Sandia National Laboratories, Matls. & Process Modlg., Albuquerque, NM 87185 USA; William John Plumbridge, Open University, Milton Keynes MK76AA UK

8:30 AM Invited
Microstructurally Informed Solder Models: *Elizabeth A. Holm*[1]; Michael K. Neilsen[2]; Arlo F. Fossum[2]; Paul T. Vianco[2]; Steve N. Burchett[2]; [1]Sandia National Laboratories, Matls. & Process Modlg., PO Box 5800, MS 1411, Albuquerque, NM 87185-1411 USA; [2]Sandia National Laboratories, PO Box 5800, Albuquerque, NM 87185 USA

Because solders operate at high homologous temperatures, microstructural evolution and cyclic strain combine to initiate thermomechanical fatigue (TMF), a principal failure mechanism in Pb-Sn solders. Since predicting interconnect lifetime is critical to improving design and reliability, we have developed a viscoplastic continuum damage (VCD) model for TMF of Pb-Sn solders that includes the coupling between microstructural evolution and thermomechanical response. In particular, the Pb-rich phase size influences local strength; the local stress, in turn, influences the coarsening rate. This model captures experimentally observed phenomena such as local coarsening near stress concentrations. Utilizing a microstructural failure criterion, we predict widely varying interconnect lifetimes for different joint geometries. A simplified version of the VCD model, the Solder Interconnect Predictor (SIP), is available for desktop systems. We are utilizing a similar approach to develop a unified creep plasticity model for Pb-free solders; preliminary results will be presented.

9:00 AM Invited
Reliability Prediction of Lead-Free Solders - Current Status and Future Challenges: *Chris John Bailey*[1]; Hua Lu[1]; Stoyan Stoyanov[1]; [1]University of Greenwich, Sch. of Computing & Math. Scis., Old Royal Naval College, Maritime Greenwich, Greenwich, London SE10 9LS England

Reliability prediction methods are now used by many organisations early in design. This paper will discuss the current status of these methods in context of the lifetime prediction of lead-free solders. Methods based on generated databases (i.e. Mil-hdbk-217), Physics-of-Failure, and others will be discussed. In particular the paper will highlight the current status of finite element modelling for fatigue life predictions of lead-free solder joints and the challenges ahead. The paper will demonstrate such prediction using current creep and damage models for Sn-Ag-Cu solder. The paper will also highlight areas in which modellers and experimentalists should work closely together to optimise the accuracy of next generation reliability predictions for pb-free solders.

9:30 AM
Role of Intergranular Microcracking in Cyclic Softening of Sn-3.8Ag-0.7Cu Alloy: *Q. L. Zeng*[2]; Z. G. Wang[2]; J. K. Shang[1]; [1]University of Illinois, Dept. of Matls. Sci. & Engrg., 1304 W. Green St., Urbana, IL 61801 USA; [2]Institute of Metal Research, Shenyang Natl. Lab. for Matls. Sci., Shenyang 110016 China

Low-cycle fatigue behavior of the Sn-Ag-Cu ternary eutectic alloy was investigated under fully reversed loading condition. The solder alloy exhibited cyclic softening early in the fatigue life and continued to soften as number of fatigue cycles increased. Following cyclic loading, numerous microcracks were found in the microstructure. Most of the microcracks were located along the grain boundaries in the areas with finer grains. The areal density of the microcracks increased with both strain amplitude and cycle number. By combining percholation theory with microcracking analysis, the cycle-dependent softening behavior was shown to result from accumulation of microcrack density with fatigue cycles.

9:55 AM
Evaluation of the Repeated Reverse Shear and Stress Relaxation Behavior of Eutectic Sn-3.5Ag Solder Joints: *Hongjoo Rhee*[1]; K. N. Subramanian[1]; Andre Lee[1]; [1]Michigan State University, Dept. of Chem. Engrg. & Matls. Sci., EB2527, E. Lansing, MI 48824-1226 USA

Solder joints experience repeated reverse straining during thermal excursions encountered in service, as a consequence of stresses that arise due to CTE mismatches between components. In order to understand the basic processes involved under such conditions, repeated reverse shear straining with associated stress relaxation at the shear strain extremes were carried out at various temperatures, with different shear strain amplitudes, after imposing different pre-strains at various pre-strain rates prior to stress relaxation events. Findings from such studies were compared with previously reported findings from monotonic shear stressing and stress relaxation tests. Residual stress during stress relaxation period decreased more rapidly under repeated reverse straining. Stress relaxation during subsequent cycles of straining depends strongly on the test temperature and the imposed strain amplitude. Work supported by the National Science Foundation under grant NSF DMR-0081796.

10:20 AM Break

10:35 AM Invited
Achieving Reliability and Structural Integrity in the Lead-Free Era: *William John Plumbridge*[1]; [1]Open University, Walton Hall, Milton Keynes MK76AA UK

The introduction of lead-free solders compounds the pressures on Designers to ensure reliability. Reliability is complex, depending on many factors that generally fall into the Manufacturing or Performance categories. For the latter, reliance on purely empirical (accelerated) testing is becoming ineffective as service conditions and performance demands become more arduous. The requirements for a paper-based design strategy, as employed in other high temperature engineering applications, are considered. Few failure modes of electronics equipment in service, such as fatigue or creep, are monomechanistic. More than one form of constitutive equation is needed to adequately describe behaviour. Modelling or computational analysis should be based on an understanding of the prevailing mechanisms and knowledge of the dominant process. Using lead-free and lead-bearing data, these arguments are considered for continuum and defect-tolerant design approaches. It is further demonstrated that the relevant mechanical properties of the lead-free solders appear at least satisfactory, although exceptions exist.

11:05 AM
Evaluation of Parameters Affecting the Service Life of Sn-Based Solder Joints Under Thermomechanical Fatigue: J. G. Lee[1]; *K. N. Subramanian*[1]; [1]Michigan State University, Chem. Engrg. & Matls. Sci., E. Lansing, MI 48824-1226 USA

A simple parametric approach to predict service life of Sn-based solder joints has been suggested. This paper evaluates the material related parameters that affect service life of Sn-based solder joints under realistic thermal excursions encountered in service by incorporating findings from studies related to material and service issues. This investigation examines the roles of these parameters and their relative importance by carrying out studies on Sn-based solder joints of realistic dimensions under realistic thermomechanical fatigue (TMF) cycling, and isothermal shear conditions. Work supported by the National Science Foundation under grant NSF DMR-0081796 and NSF DMI-0339898.

11:30 AM
Recent Experiments on the Thermomechanical Response of an Adaptive Lead-Free Solder: Zhixiang Wang[1]; *Bhaskar S. Majumdar*[1]; Indranath Dutta[2]; [1]New Mexico Tech, Matls. Dept., 801 Leroy Place, Socorro, NM 87801 USA; [2]Naval Postgraduate School, Ctr. for Matls. Sci., Mechl. Engrg. Dept., Monterey, CA 93943 USA

In an effort to improve the thermomechanical fatigue (TMF) life of lead-free solders in flip chip applications, we have been experimenting with the use of a NiTi shape memory alloy as a reinforcing phase. The conceptual framework is that the soft martensite phase of the alloy would deform along with the solder, but its transformation into the austenite phase at an elevated temperature would induce a backstress on the solder, in the form of a transformation induced eigenstrain. This would reduce the overall creep strain of the solder in the temperature regime when the base solder has very low resistance to deformation. Our experiments were conducted on a Sn-3Ag solder alloy, and we have utilized a single NiTi fiber composite under double shear loading to test the performance and feasibility of this adaptive compositing approach. Both mechanical TMF data as well as microstructural stability issues of the composite will be presented. The test data will be compared with predictions of our model using an Eshelby approach. Some recent results from NiTi particle-reinforced Sn-3Ag solder will also be presented, to illustrate the overall performance of this system in ball grid array applications. We acknowledge support by the Army Research Office with Dr. David Stepp as the program monitor.

11:55 AM
Mechanical Fatigue Properties of Through-Hole Joints at Elevated Temperature: Yoshiharu Kariya[1]; *Tomokazu Niimi*[1]; Kengo Mitose[2]; Takao

Hashiguchi[2]; Tadatomo Suga[3]; [1]National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044 Japan; [2]Furukawa Electric Co., Ltd., 2-4-3 Okano, Nishi-Ku, Yokohama 220-0073 Japan; [3]University of Tokyo, Dept. of Precision Engrg., 7-3-1 Hongo, Bunkyo-Ku, Tokyo 113-8656 Japan

The through-hole technology is still used for the application that requires high reliability such as automobile under hood. However, scientific researches on a mechanical reliability of the through-hole joints were not enough performed to date, although voluminous studies on the reliability for the SMT joints was made to implement of lead free soldering. In addition, mechanical reliability of the solder joints at a temperature over 398K was not well understood, as most accelerating tests are conducted a below 373K temperature. In this study, a mechanical fatigue testing method was proposed to evaluate fatigue endurance of the through-hole joints, and was performed at 413K to investigate fatigue damage of the joints made with Sn-3Ag-0.5Cu lead-free solder. Details of the fatigue life and fatigue damage of the through-hole joints at 413 K will be presented in comparison with the damage at room temperature.

The Accelerated Implementation of Materials & Processes: Mechanical Property Modeling - Superalloys

Sponsored by: TMS - Structural Materials Division, TMS - ASM/MSCTS-Thermodynamics & Phase Equilibria Committee, TMS - EMPMD/SMD-Chemistry & Physics of Materials Committee, TMS - MPMD-Computational Materials Science & Engineering-(Jt. ASM-MSCTS)
Program Organizers: Rollie E. Dutton, Air Force Research Laboratory, AFRL/MLLMP, WPAFB, OH 45433 USA; John E. Allison, Ford Motor Company, Materials Science and Advanced Engineering, Dearborn, MI 48124-2053 USA; John J. Schirra, Pratt & Whitney, East Hartford, CT 06108 USA; Axel van de Walle, Northwestern University, Materials Science and Engineering, Evanston, IL 60208-3108 USA

Wednesday AM — Room: Mardi Gras Ballroom H
September 29, 2004 — Location: Marriott New Orleans Hotel

Session Chair: Axel van de Walle, Northwestern University, Matls. Sci. & Engrg., Evanston, IL 60208-3108 USA

8:30 AM
Multiscale Modeling Challenges in Predicting the Microstructure-Dependent Mechanical Performance of Superalloys: *Dennis M. Dimiduk*[1]; T. A. Parthasarathy[2]; S. I. Rao[2]; Yoon-Suck Choi[2]; M. D. Uchic[1]; [1]Air Force Research Laboratory, AFRL/MLLM Bldg. 655, 2230 Tenth St., Wright-Patterson AFB, OH 45433-7817 USA; [2]UES, Inc., AFRL/MLLM, 4401 Dayton-Xenia Rd., Dayton, OH 45432-1894 USA

This presentation briefly reviews a simulation and testing methodology developed through the DARPA Accelerated Insertion of Materials initiative. The new methodology builds upon a multitude of rapid microstructural and property assessments of selected local regions of a material (i.e. single-crystal regions, defected regions, grain aggregates, etc.). The selected regions can be from a fully-processed component or from materials specifically prepared to represent selected aspects of the full-scale process. The results from these assessments are used to define parameters within a hierarchy of mathematical and numerical representations of the material, and this information may be used in design performance simulation codes to predict the intrinsic response of larger-scale structures. In so doing, the methodology incorporates the influence of the local, microscopic and submicroscopic heterogeneous nature of structural materials and their properties directly into design procedures. Further, the methodology may be used to anticipate the effects of defects on the performance of the full-scale structure. While most steps of this alternative design and test methodology, are amenable to automation, building and validating the framework of simulation codes and test methodologies is not. Thus, selected challenges in defining and implementing the multiscale modeling framework for superalloys, together with progress toward meeting them, will be shown. As a whole the new methodology will reduce the number of iterative large-scale cycles required to qualify a material's suitability for structural service; thus, the new method is a framework for accelerating the development of structural materials.

8:55 AM
Microstructural Characterization of Nickel-Based Superalloys: *E. Sarath K. Menon*[1]; Michael Uchic[2]; Dennis M. Dimiduk[2]; [1]UES Inc., Matl. Processes Div., 4401 Dayton-Xenia Rd., Dayton, OH 45432-1894 USA; [2]Air Force Research Laboratory/MLLM, Wright-Patterson AFB, OH 45433-7817 USA

Nickel-based superalloys find extensive use in high-temperature applications. A large number of the alloys used rely on carefully tailored compositions and heat-treatment schedules that result principally in a microstructure constituted of the ordered γ' phase ($L1_2$ crystal structure) distributed in a γ (FCC crystal structure) matrix. Indeed, the optimization of the requisite properties is achieved by a combination of grain size control, distribution of minority phases such as carbides and borides and most importantly a multi-sized distribution of the γ' phase. Needless to say, a precise knowledge of the uniformity of distribution of the phases, their average sizes as well as their size distribution is essential in evaluating the properties associated with various heat-treatments. This presentation shows results from SEM and TEM methods used to characterize the microstructures in two alloys, IN100 and René88DT, and the subsequent quantitative parameters obtained, such as volume fraction, average size and size distribution of the γ' phase. The use of back-scattered electron imaging in the SEM from thin-foil sections is shown to provide high-quality micrographs suitable for accurate quantification of the larger-sized γ phase (greater than ~50nm), and this technique will be demonstrated. Micro-analytical information obtained from both the γ and the γ' phases through TEM-EDS analysis also will be presented. Work performed under USAF Contract #F33615-01-5214.

9:20 AM
Discrete Dislocation Simulations of Precipitation Hardening in Superalloys: *Satish I. Rao*[1]; T. A. Parthasarathy[1]; D. M. Dimiduk[2]; Peter M. Hazzledine[1]; [1]UES Inc., Matls. & Processes, 4401 Dayton-Xenia Rd., Dayton, OH 45432-1894 USA; [2]Air Force Research Laboratory/MLLM, Wright-Patterson AFB, OH 45433 USA

A mesoscopic dislocation simulation is described that measures the critical resolved shear stress of an alloy strengthened by concentrated ordered coherent precipitates. The low-temperature, low-strain strengthening mechanisms in a model representation of a Ni-based superalloy, containing a high volume fraction of Ni_3Al precipitates (γ'), has been studied by using discrete dislocation simulations. Superalloys are strengthened by many effects, including the crystallographic order in the γ' phase, solution hardening in γ -phase matrix and γ' phase and coherency stresses (principally in γ-phase). In the model, a pair of screw or 60° a/2<110> character dislocations was made to glide under external stress on an octahedral plane of γ-phase, intersected by a random distribution of spherical or cubic γ' precipitates. The applied stress was raised until the dislocations could defeat (cut or bow round) all the obstacles. By performing a large number of simulations, the effects of size, shape, volume fraction, coherency strain and antiphase boundary (APB) energy of γ' (within the ranges of industrial interest) were studied. The discrete dislocation simulation results on precipitation hardening in a Ni-based superalloy are discussed in the talk and compared with classical analytical predictions. Worked performed under USAF Contract F33615-01-C-5214.

9:45 AM Break

10:00 AM
Transformation Kinetics of Fine γ' Precipitates in Rene 88 DT: *Peter Maxwell Sarosi*[1]; Gopal Babu Viswanathan[1]; Deborah Whitis[2]; Michael J. Mills[1]; [1]Ohio State University, Matls. Sci. & Engrg., Columbus, OH 43210 USA; [2]GE Aircraft Engines, Matls. & Processes Engrg. Dept., Cincinnati, OH USA

Nickel-based superalloys that contain multi-modally distributed γ' in a γ matrix offer the best combinations of mechanical properties. This is also the case for Rene 88 DT, a proprietary engineering alloy used in turbine disk components. In particular, the volume fraction and size of the finest (tertiary) γ' precipitate distributions (down to 3nm) may significantly affect the creep properties. Importantly, it has been posited that microstructural changes - particularly with regards to tertiary precipitates - during creep at the same stress and temperature may alter the preferred creep deformation mechanisms during creep. Furthermore, since ageing degrades the creep properties it is important to determine the microstructural stability (transformation kinetics) at service temperatures (700°C) particularly with regards to the tertiary γ' precipitates. Initial results from computer models already predict the precipitation and transformation kinetics of γ' in Rene 88 DT but require validation from experimental data taken from this study. Therefore, an investigation of the transformation kinetics of the γ' precipitates was undertaken using samples that were isothermally aged at 700°C for different ageing times (0 hours to 1050 hours) and samples subjected to continuous cooling (75°F/min to 400°F/min). Precipitate sizes and volume fractions of both tertiary and the larger secondary γ' distributions were determined by analyzing images obtained using Energy Filtered Transmission Electron Microscopy and conventional SEM imaging. The results were analyzed and compared with computer models.

10:25 AM
Role of Temperature on the Creep Deformation Mechanisms of Nickel Based Superalloy Rene 104: *Raymond R. Unocic*[1]; Peter M. Sarosi[1]; G.

Babu Viswanathan[1]; Michael J. Mills[1]; [1]Ohio State University, Matls. Sci. & Engrg., 477 Watts Hall, 2041 College Rd., Columbus, OH 43210 USA

The nickel-based superalloy Rene 104 has been developed as an alternative disk alloy material for gas turbine engine applications that require a high temperature structural material with exceptional creep resistance. The creep response of these alloys have been evaluated through constant stress creep tests performed under a matrix of temperatures (1250-1500°F) and stress levels (50-100ksi). The creep deformation structures of these alloys were subsequently investigated using transmission electron microscopy (TEM). The temperature at which these materials were crept revealed a notable influence on the deformation characteristics. In the lower temperature regime, the dominant deformation mechanism was found to be that of microtwinning. Characteristic of this regime are continuous faults that pass through the precipitates as well as the matrix. High-resolution transmission electron microscopy (HREM) proved that the faults are indeed microtwins. The mechanisms by which these structures are formed are to be discussed. In the higher temperature regime, there is evidence of 1/2<110> type matrix dislocations by-passing precipitates as well as precipitate shearing which leaves behind isolated faults about larger secondary g' precipitates. The deformation characteristics between the two temperature regimes gives a clear distinction between deformation mechanisms. A possible model emphasizing the role of temperature on thermally activated deformation processes that illustrates the transition between microtwinning, precipitate shearing, and bypassing will be discussed.

10:50 AM

Creep at Intermediate Temperatures in the Ni-Based Superalloy Rene 88DT: *Gopal B. Viswanathan*[1]; Peter M. Sarosi[1]; Michael F. Henry[2]; Deborah Whitis[3]; Michael J. Mills[1]; [1]Ohio State University, Matls. Sci. & Engrg., 477 Watts Hall, 2041 College Rd., Columbus, OH 43210 USA; [2]GE Global Research Center, Schenectady, NY USA; [3]GE Aircraft Engines, Matls. & Processes Engrg. Dept., Cincinnati, OH USA

Creep strength in Ni-base superalloys depends on a number of interrelated microstructural parameters, including the volume fraction, particle size, distribution, and chemical characteristics of the gamma prime (Ni3Al type) precipitates that are present in FCC g matrix. At intermediate temperatures i.e. 650-800°C (depending on the alloy), deformation is extremely planar and complex. The mechanisms responsible for deformation at these temperatures is much less clear and more importantly the effect of microstructure and applied stress is not fully understood. In this study, the dislocation substructures developed after small-strain (0.5%) creep at 650°C and at stress levels in the range from 115-140 ksi, in Rene 88 DT have been analyzed using conventional and high resolution transmission electron microscopy. Clear differences in creep strength and substructures have been observed for samples heat treated with two different cooling rates from the supersolvus heat treatment temperature. For the more rapidly cooled (400°F/min) and finer microstructure exhibits very low initial creep rates, and deformation microtwinning is the dominant deformation process. For the more slowly cooled (75 °F/min) and coarser microstructure, the creep rates are much faster, and isolated faulting of individual secondary gamma prime precipitates is observed. The detailed dislocation analyses leading to these conclusions will be presented. The transition from the isolated faulting mechanism in coarser the gamma prime microstructure to microtwinning in the finer ggamma prime microstructure is attributed to the effect of the volume fraction of the tertiary gamma prime precipitates on the stress required to drive 1/2<110> versus 1/3<112> dislocations through the matrix and tertiary particles. A simple model predicting this transition in mechanism will be discussed, as will the possible rate-limiting processes for these two deformation modes.

The Effects of Microstructure and Property Homogeneity/Variability on Product Performance: Session II

Sponsored by: AIST, AIST - Division VI
Program Organizers: J. M. Rodriguez-Ibabe, CEIT Spain; Roger Pradhan, ISG Reseach; AIST Staff, Association of Iron Steel Technology, Warrendale, PA 15086 USA

Wednesday AM — Room: Grand Ballroom M
September 29, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Craig V. Darragh, The Timken Company, Canton, OH USA; Amy J. Bailey, TXI- Chaparral Steel, Midlothian, TX 76065 USA

8:30 AM

Laser Ultrasonic Monitoring of Recrystallization of Steels: *Silvio E. Kruger*[1]; Guy Lamouche[1]; André Moreau[1]; Jean-Pierre Monchalin[1]; Matthias Militzer[2]; [1]National Research Council of Canada, Indust. Matls. Inst., 75, Boul. de Mortagne, Boucherville J4B6Y4 Canada; [2]University of British Columbia, The Ctr. for Metallurgl. Process Engrg., Vancouver, BC V6T 1Z4 Canada

Laser-ultrasonics is a non-destructive and non-contact technique that allows ultrasonic assessment of some materials characteristics, like grain size, phase fraction and texture. The suitability of this technique has been demonstrated already in metals processing environments. In this paper, ultrasonic velocity and absorption are measured during annealing of steels (low carbon and IF) in a furnace. Velocity variations due to changes in texture during recrystallization are sensitive to recrystallization stages as measured by metallographic and texture measurements. The absorption (or internal friction) of ultrasonic waves is also shown to be sensitive to annealing. The absorption increases during annealing in steels due to an increase of the magnetoelastic damping. The use of the technique for real-time monitoring of recrystallization in continuous annealing production lines as a sensor for feeding a closed-loop control of processing parameters and its impact on reducing product variability is discussed.

9:00 AM

Abnormal Grain Growth During Thermomechanical Processing of Ti Microalloyed Medium Carbon Steels: *Jose M. Rodriguez-Ibabe*[1]; R. Bueno[1]; A. Echeverria[1]; B. Lopez[1]; [1]CEIT and Tecnun, P. M. Lardizabal 15, San Sebastian 20018 Spain

Microalloyed forging steels, mainly based on Ti and Ti-V microadditions, are characterized by refined ferrite-pearlite room temperature microstructures comparing to plain C-Mn steels. The level of strength and toughness that can be reached with these materials is in most cases adequate, however they are susceptible of showing microstructure heterogeneities that can significantly impair toughness behaviour. Consequently, new applications of these microalloyed steels are subjected to the improvement in the microstructure homogeneity. This work analyses the behaviour of three medium carbon steels (C-Mn, Ti-V and Ti-B) by performing torsion tests at deformation conditions similar to those used in hot forging. The results show that the austenite mean grain size is notably refined by Ti microaddition, however, following deformation abnormal grain growth phenomena have been identified. The evolution of the coarser grains present in the microstructures has shown to be dependent on the steel and deformation conditions.

9:30 AM Break

10:00 AM

Laser Ultrasonic Sensor for On-Line Steel Tubing Process Control: *Silvio E. Kruger*[1]; Gerald Jeskey[2]; Robert Kolarik[3]; E. Buddy Damm[3]; Jean-Pierre Monchalin[1]; Guy Lamouche[1]; Marc Choquet[4]; [1]National Research Council of Canada, Indust. Matls. Inst., 75, Boul. de Mortagne, Boucherville, Québec J4B6Y4 Canada; [2]Jeskey Consulting; [3]The Timken Company; [4]Tecnar Automation

The seamless tube making process oftentimes causes wall thickness variations along the tube length. A laser-ultrasonic system was developed in a project done under a partial funding award from the U.S. Department of Energy. The system which consists of generation and detection lasers and an interferometer located in a cabin outside the tube mill, and a fiber-coupled inspection head located above the process line, was installed immediately after the final operation in tube making. Tube wall thickness and eccentricity measurements are used to guide mill adjustments to achieve the desired tolerances. Over 600,000 tubes were inspected in the first 18 months of operation. The austenitic grain size of in-process steel tubing is important due to its impact on the mechanical properties of the final product. In a separate effort, the functionality to sense grain size was added to the system using the same signals that measure the tube wall thickness.

10:30 AM

A Diffusion Model for the Influence of Oxygen and Sulfur on the Non-Equilibrium Distribution of Chromium in Austenitic Stainless Steel Welds and Slabs: *Michael F. McGuire*[1]; [1]McGuire Associates, 2901 Smallman St. 5a, Pittsburgh, PA USA

Research has shown that austenitic stainless steels sometimes display chromium depletion around sulfide inclusions. A model is presented which shows that the precipitation location and kinetics of the interstitial solutes, sulfur and oxygen, can produce this chromium depletion and can account for the observed susceptibility to pitting corrosion. The model also describes the conditions under which the precipitation occurs at grain boundaries and the hot working defects which can result. The dependence of both pitting susceptibility and tendency toward sliver-type defects on key processing and material variables is discussed. The parallels between sensitization and pitting are discussed and countermeasures are proposed.

11:00 AM

Effects of Microstructural Variability on Fatigue Life Prediction of Martensitic 17-4PH Steel: *Animesh Dey*[1]; Robert G. Tryon[1]; Vikram

Bhamidipati[1]; [1]VEXTEC Corporation, 750 Old Hickory Blvd., Bldg.-2, Ste. 270, Brentwood, TN 37027 USA

An important aspect of fatigue failures in steel structures is that large variations in the lifetime of the components are observed. Such variability can be attributed to the significant variation observed in the microstructural makeup of steels such as martensitic 17-4PH. VEXTEC has been developing new and innovative methods to understand and predict when fatigue failure will occur. The methods are aimed at predicting the variation in fatigue life based on the statistical variation of the microscopic structure of the material. Material parameters at metallic grain level, such as texture and orientation, variation in grain size due to processing, variation in grain boundary strength, etc., are used along with fundamental physics-based models to predict the damage as it accumulates. The methods are based on probabilistic mesomechanics and use a virtual prototyping technique relying on computer simulation of real material behavior.

Titanium for Healthcare, Biomedical, and Dental Applications: Composites and Coatings

Sponsored by: TMS - Structural Materials Division, Japan Institute of Metals, TMS - SMD-Titanium Committee, TMS - SMD-Corrosion and Environmental Effects Committee-(Jt. ASM-MSCTS)

Program Organizers: Carl Boehlert, Alfred University, School of Ceramic Engineering and Materials Science, Alfred, NY 14802 USA; Dhanesh Chandra, University of Nevada, Metallurgical and Materials Engineering, Reno, NV 89557 USA; Masahiko Ikeda, Kansai University, Department of Materials Science and Engineering, Suita, Osaka 564-8680 Japan; Mitsuo Niinomi, Toyohashi University of Technology, Department of Production Systems Engineering, Toyohashi 441-8580 Japan

Wednesday AM — Room: Mardi Gras Ballroom D
September 29, 2004 — Location: Marriott New Orleans Hotel

Session Chair: Daniel B. Miracle, Air Force Research Laboratory, Matls. & Mfg. Direct., Wright Patterson AFB, OH 45433 USA

8:30 AM Invited

Affordable Thermomechanical Processing of Titanium Alloys: S. Tamirisa[2]; R. B. Bhat[3]; D. McEldowney[4]; *D. B. Miracle*[1]; [1]Air Force Research Laboratory, Matls. & Mfg. Direct., 2230 Tenth St., Wright-Patterson AFB, OH 45433 USA; [2]Ohio University, Athens, OH 45701 USA; [3]UES, Inc., 4401 Dayton-Xenia Rd., Dayton, OH 45432 USA; [4]University of Dayton, Dept. of Matls. Sci. & Engrg., Dayton, OH 45469 USA

A significant international effort is now underway to dramatically decrease the primary reduction cost for titanium. However, ingot breakdown and billet conversion can require up to 24 hours of intensive thermomechanical processing, involving multi-step deformations with narrow processing windows, and can account for up to 30-40% of mill product cost. Thus, innovative approaches to reduce the cost of thermomechanical processing provide an important opportunity for improving the affordability of titanium alloys. Titanium alloys with small boron additions (typically less than 1 wt%) are established in automotive components and are being studied for dental applications. Boron is a potent grain refiner and grain stabilizer, eliminating grain growth up to 150°C above the beta transus and producing fine-grained equiaxed microstructures after cooling from temperatures as high as 1150°C. Thus, fine-grained microstructures can be achieved in boron-modified titanium alloys with dramatic reductions in the thermomechanical processing currently required for conventional titanium alloys. The results of studies to define the influence of boron additions in producing significant reductions in thermomechanical processing and improved superplastic forming will be presented and discussed.

8:55 AM

Thermo-Mechanical Processing of Cast Ti-B Alloys: *Sesh Tamirisa*[1]; Radhakrishna B. Bhat[2]; Dale J. McEldowney[3]; Daniel B. Miracle[4]; [1]Ohio University, Mechl. Engrg., AFRL/MLLMD, 2230 Tenth St., Bldg. 655, Ste. 1, Wright-Patterson AFB, OH 45433 USA; [2]UES, Inc., Matls. Procg., 4401 Dayton-Xenia Rd., Dayton, OH 45432 USA; [3]SOCHE, AFRL/MLLMD 2230 Tenth St., Wright-Patterson AFB, OH 45433 USA; [4]Air Force Research Laboratory, MLLMD, AFRL/MLLMD, 2230 Tenth St., Wright-Patterson AFB, OH 45433 USA

The stiffness and strength of conventional titanium alloys can be significantly enhanced by the addition of boron while retaining useful fracture properties. These improvements are due to the formation of fine in situ TiB precipitates in the alloy for boron concentrations as low as 0.01 wt.%. It has been demonstrated that boron can simply be added as an additional alloying element to the melt and conventional casting practices can be used to produce affordable Ti-B alloys. In this presentation, we describe the thermo-mechanical response of various cast Ti-B alloys. The presence of TiB influences the kinetics of beta to alpha phase transformation during cooling from the beta phase field across the beta transus. The TiB precipitates induce heterogeneous nucleation of the alpha phase and produce fine-grained equiaxed microstructures even without imposing plastic deformation. The ability to obtain grain refinement and microstructural conversion by boron addition significantly reduces or eliminates several ingot breakdown and billet conversion processing steps currently necessary for titanium alloys. During processing in the beta phase field, the TiB restricts the beta grain growth and stabilizes fine-grained equiaxed microstructure. This remarkable ability to retain fine-grained microstructures in the monolithic beta phase field enables novel beta processing methods including superplasticity at faster deformation rates. Optimization of processing parameters to obtain controlled microstructures in Ti-B alloys and the ability to shape-form these materials using conventional metalworking processes will be discussed.

9:20 AM

Microstructures and Mechanical Properties of Cast Titanium Alloys Modified with Boron: *Radhakrishna B. Bhat*[1]; Sesh Tamirisa[2]; Dale J. McEldowney[3]; Vilupanur A. Ravi[4]; Jaimie S. Tiley[5]; Daniel B. Miracle[5]; [1]UES Inc., Matls. & Processes, 4401 Dayton-Xenia Rd., Dayton, OH 45432 USA; [2]Ohio University, Mechl. Engrg., Athens, OH 45701 USA; [3]University of Dayton & SOCHE, Dayton, OH 45469 USA; [4]Calpoly, Chem. & Matls. Engrg., Pomona, CA 91768 USA; [5]Air Force Research Laboratory, Matls. & Mfg. Direct., Wright-Patterson AFB, Dayton, OH 45433 USA; [5]Air Force Research Laboratory, Matls. & Mfg. Direct., Wright-Patterson AFB, Dayton, OH 45433 USA

Titanium alloys modified with small boron additions have been successfully transitioned to automotive applications and are being actively considered for insertion in other areas including armor, aerospace and dental. Boron additions to titanium results in the formation of in situ TiB precipitates which improve both the specific strength and stiffness of the alloy. In addition, TiB precipitates also induce significant microstructural refinement in the as-cast Ti alloys improving the ductility. Various levels of boron in the range 0.02-1.0 wt.% were added to CP titanium, Ti-6Al-4V, and Ti-6Al-2Sn-4Zr-2Mo-0.1Si alloys during melting and were cast into billets of 70 mm diameter and 500 mm length. The microstructure and tensile properties in both longitudinal and transverse orientations of the as-cast Ti-B alloys will be presented. Microstructure-property correlations and the influence of TiB on the matrix microstructure evolution will be discussed.

9:45 AM

Characterization and Thermal Stability of TiB in Ti-6Al-4V-1.6B Alloy: *Dale Joseph McEldowney*[1]; S. Tamirisa[2]; R. B. Bhat[3]; D. Eylon[4]; D. B. Miracle[5]; [1]University of Dayton/SOCHE, 300 College Park, Dayton, OH 45469 USA; [2]Ohio University, Mechl. Engrg., Athens, OH 45701 USA; [3]UES Inc., Dayton, OH 45432 USA; [4]University of Dayton, Matls. Engrg., 300 College Park, Dayton, OH 45469 USA; [5]Air Force Research Laboratory, Matls. & Mfg. Direct., Wright-Patterson AFB, OH 45431 USA

Recent studies on boron additions to titanium alloys have shown very promising results with increases in strength and stiffness of 60-70% in comparison to titanium alloys without boron. Utilizing a prealloyed (PA) powder metallurgy approach, Ti-6Al-4V-1.6B alloy was produced and subjected to further thermo-mechanical processing via blind die compaction and round-to-round extrusion. The extruded material had an equiaxed-alpa microstructure with about 10 vol% finely dispersed TiB precipitates. The TiB precipitates were in the form of needles with the highest percentage generally 2-5 um in diameter and aspect ratio of about 10. A lower fraction of TiB needles was also present with a diameter range of 30-50 nm and similar aspect ratio. The improved strength and stiffness of these Ti-B alloys is a function of the volume fraction, size and orientation of the TiB needles. Hence, it is important to establish the stability of these needles under thermal exposure. The thermal stability of the TiB phase has been measured and the size and morphology of the TiB is reported as a function of temperature and time of thermal exposure. Different rate-controlling mechanisms that operate in the alpa+beta and beta phase regions are identified using coarsening models.

10:10 AM Break

10:20 AM

Functionally Gradient Diamondlike Carbon Thin Films on Ti-6%Al-4%V Alloy: *Roger J. Narayan*[1]; [1]Georgia Institute of Technology, Matls. Engrg., 771 Ferst Dr. NW, Atlanta, GA 30332-0245 USA

Diamondlike carbon (DLC) is an amorphous form of carbon with a high fraction of sp^3 hybridized carbon. DLC thin films possess exceptional biocompatibility, wear resistance, and corrosion resistance. Unfortunately, conventional DLC films demonstrate poor adhesion to medical metals and polymers. In this work, self-assembled functionally gradient DLC-metal nanocomposite films of ~1 micron thickness were deposited on Ti-6%Al-4%V substrates. Film microstructure was characterized using transmission electron microscopy, electron energy loss spectroscopy, and Raman spectroscopy. Scratch testing demonstrated good adhesion of the DLC-metal nanocomposites to Ti-6%Al-4%V. Wear testing using a CSM linear tribometer demonstrated wear life in excess of 300,000 cycles for tests conducted in Ringer's USP solution. These novel DLC-metal films have numerous potential medical applications.

10:45 AM
Hydroxyapatite-Diamondlike Carbon Nanocomposite Films on Ti-6%Al-4%V Alloy: *Roger Jagdish Narayan*[1]; [1]Georgia Institute of Technology, Matls. Engrg., 771 Ferst Dr. NW, 0245, Atlanta, GA 30332-0245 USA

Hydroxyapatite is a bioactive ceramic that mimics the mineral composition of natural bone. Conventional plasma-sprayed hydroxyapatite coatings demonstrate poor adhesion and poor mechanical integrity. We have developed a novel multiple target pulsed laser deposition technique using to create hydroxyapatite- diamondlike carbon nanocomposite coatings on Ti-6%Al-4%V alloy. The diamondlike carbon interlayer serves to prevent metal ion release and improve adhesion of the hydroxyapatite coating. Diamondlike carbon is an amorphous, hydrogen-free, and sp^3-hybridized form of carbon that exhibits exceptional biocompatibility, wear resistance, and corrosion resistance. The films were characterized using SEM, TEM, XRD, Raman spectroscopy, and mechanical testing. Hydroxyapatite-diamondlike carbon bilayers demonstrate promise for use in several orthopaedic implants.

11:10 AM
Calcium-Deficient Hydroxyapatite Coating on Nano-Tube Arrays of Anodized Titanium: *Krishnan Selva Raja*[1]; K. Paramguru[1]; Manoranjan Misra[1]; [1]University of Nevada, Metallurgl. & Matls. Engrg., MS 388, Reno, NV 89557 USA

Calcium-deficient hydroxyapatite (CDHA) with a Ca/P ratio closer to 1.5 resembles bone mineral both structurally and compositionally. Electrochemical deposition of CDHA is being carried out on anodized titanium. Regular arrays of nanotube structure of titania resulted in a nanocrystalline apatitic coating on titanium substrate. Diameter and length of the titania nanotubes are optimized to obtain a higher bond strength by controlling both the anodization and deposition parameters. The effect of crystal structure of the titania tubes (amorphous vs anatase) on bonding characteristics is also being studied. Multi step-multi voltage anodization of titanium is being carried out in different electrolytes in order to obtain inter connected nano-pores with varying pore density across the thickness of the oxide layer. This type of nanotube configuration can be used for insitu drug delivery system.

11:35 AM
Interconnected Titanium/UHMWPE Biocomposites: P. L. Liu[1]; *J. K. Shang*[1]; [1]University of Illinois, Dept. of Matls. Sci. & Engrg., 1304 W. Green St., Urbana, IL 61801 USA

Titanium and its alloys are widely used in orthopedic applications where stress shielding arises because of the poor elastic mismatch between titanium and tissue. In study, interconnected Ti/UHMWPE composites were investigated to address the elastic mismatch. The composites were made by a vacuum extrusion process in which the UHMWPE powder was extruded into open-cell titanium foams at elevated temperatures. High pressures were applied at the last stage of the extrusion processing to ensure Ti foams were fully filled and the UHMWPE was well sintered. The mechanical properties of the composites were studied under compression. While the titanium foams had low strengths and moduli than the theoretical prediction, the composites showed greatly improved mechanical properties.

3-Dimensional Materials Science: Mathematical Representation

Sponsored by: TMS - Structural Materials Division
Program Organizers: Marc J. De Graef, Carnegie Mellon University, Department Material Science & Engineering, Pittsburgh, PA 15213-3890 USA; Jeff P. Simmons, Air Force Research Laboratory, Materials & Manufacturing Directorate, Dayton, OH 45433 USA; George Spanos, Naval Research Laboratory, Physical Metallurgy Branch, Washington, DC 20375-5000 USA; Jonathan E. Spowart, UES Inc., Dayton, OH 45432 USA

Wednesday PM	Room: Mardi Gras Ballroom F/G
September 29, 2004	Location: Marriott New Orleans Hotel

Session Chairs: Anthony D. Rollett, Carnegie Mellon University, Dept. of Matls. Sci. & Engrg., Pittsburgh, PA 15213-3890 USA; Jeff Simmons, Air Force Research Laboratory, Matls. & Mfg. Direct., Wright-Patterson AFB, OH 45433 USA

2:00 PM Invited
Computer Simulations of "Realistic" Material Microstructures: *Arun M. Gokhale*[1]; Harpreet Singh[1]; Yuxiong Mao[1]; [1]Georgia Institute of Technology, Matls. Sci. & Engrg., 771 Ferst Dr., Atlanta, GA 30332-0245 USA

An important inverse problem in the development of microstructure representation methodologies is that once a microstructure is quantified in detail, using those data is it possible to simulate a microstructure that is statistically similar to the corresponding real microstructure in its geometric attributes including spatial arrangement (clustering, etc.) of the features? If this is possible, then the simulation parameters can represent the useful geometric information concerning the real microstructure. We present a technique for simulations of microstructures of discontinuously reinforced aluminum alloy (DRA) matrix composites such that simulated microstructures have the same complex particle morphologies, volume fraction, size distribution, and spatial clustering of the particles as in the corresponding real microstructures. This research is supported through AFOSR grant F49620-01-0045 (Dr. C.S. Hartley, Program Manager). The financial support is gratefully acknowledged.

2:30 PM Invited
Texture Analysis Using Wavelet Packets with an Artificial Neural Network Based Criterion: *Hiroyuki Yoshida*[1]; [1]University of Chicago, Dept. of Radiology, 5840 S. Maryland Ave., MC2026, Chicago, IL 60637 USA

Surface textures may be used to distinguish features of interest within an image. This is particularly useful in determining benign from malignant tumors when ultrasound imaging is used. "Echo-texture patterns" on ultrasound images are represented by spatially distributed variation of pixel values that is highly scale-dependent. We thus developed a multiscale wavelet method that can optimally classify benign from malignant tumors, based on wavelet packets and an artificial neural network. The novelty of our method is that, for any given classifier that provides a scalar measure of discrimination performance (class separability), we can automatically generate a set of orthogonal multiscale features that maximize the performance of the classifier. The general framework of our multiscale echo-texture analysis method will be described along with its application to the classification between benign and malignant liver tumors in B-mode ultrasound images.

3:00 PM
Principal Component Analysis as a Means of Representing Microstructural Information: *Jeff P. Simmons*[1]; Dennis M. Dimiduk[1]; [1]Air Force Research Laboratory, Matls. & Mfg. Direct., AFRL/MLLMD, 2230 Tenth St., Wright-Patterson AFB, Area B, Dayton, OH 45433 USA

The rise of the computer promises to accelerate the materials development process through applications of technologies that produce datasets with a richness never before realized. Image processing and similar data reduction techniques have been developed that can reduce microstructural information to quantitative metrics that can be used for automated feature recognition and decision making as well as communication between computerized techniques. While being a significant step forward, simple reduction to generic descriptors will not take advantage of the full richness of the dataset. Alternatively, we have proposed approaches that involve statistical modeling of the microstructure to produce a representation containing all typical characteristics associated with the microstructure. To this end, we have used Principal Component Analysis (PCA) on idealized microstructures to reduce the representation to a small number of basis functions. The statistical properties of the expansion coefficients allow the microstructure to be represented mathematically and allows the full richness of a dataset of images to be preserved. This presentation will discuss the successes as well as the weaknesses found with this approach.

3:20 PM Break

3:40 PM Invited

On the Characterization of Grain Anisotropy: *Craig S. Hartley*[1]; Jonathan E. Spowart[2]; [1]Air Force Office of Scientific Research, Aeros. & Matls. Sci., 4015 Wilson Blvd., Rm. 713, Arlington, VA 22203 USA; [2]UES, Inc., 4401 Dayton-Xenia Rd., Dayton, OH 45432 USA

The mechanical behavior of materials subjected to three-dimensional states of stress depends not only on the content and character of internal interfaces but also on the orientation of the interfaces with respect to principal axes of stress. It is necessary to characterize the spatial anisotropy of interface networks in a fashion that will permit the character and degree of the anisotropy to be included in constitutive relations relating stress to material response. This research concentrates on the spatial anisotropy of internal interface networks and its variation with simple metal forming processes. Grain shape anisotropy, characterized by a 3-D Orientation Distribution Function (ODF) that measures the spatial variation of the density of intercepts of test lines with grain boundaries, has been measured in single-phase titanium and iron alloy specimens after warm rolling and isothermal upset forging. Automated serial sectioning was used to reconstruct the 3-D microstructural features of interest. Two-dimensional stereological probes were then used to interrogate the 3-D data-sets, and obtain data for intercept densities within the deformed material at various orientations of the test probes. It is demonstrated that for these processes, the anisotropy of the grain boundary network can be described by a quadratic expression for the ODF of intercepts. The coefficients in this expression can be related to measures of bulk strain in regions where the deformation is relatively uniform. Results of this analysis, including local finite strains, are compared with total strains obtained via Finite Element Modeling of the same processes, using a simple continuum plasticity approach.

4:10 PM

The 3D Microstructure Builder: *Anthony D. Rollett*[1]; David Saylor[2]; Abhijit Brahme[1]; Joseph Fridy[3]; Sukbin Lee[1]; [1]Carnegie Mellon University, Matls. Sci. & Engrg., 5000 Forbes, Pittsburgh, PA 15213 USA; [2]Food & Drug Administration, 5600 Fishers Ln., Rockville, MD 20857-0001 USA; [3]Alcoa Technical Center, 1 Tech. Dr., Alcoa, PA 15069 USA

A set of tools is described for generating numerical three-dimensional microstructures based on experimental measurements using automated electron back-scatter diffraction on orthogonal sections. The microstructures currently allow grain shape, texture and grain boundary character (as embodied in the misorientation distribution) to be matched to the measurements in a single phase material. The discretization of the microstructure can be realized by either a Voronoi tessellation or on a regular grid (voxels on a cubic lattice). Extensions of the method are described that permit finite element meshes to be generated from the tessellations. Further extensions are described that permit two-phase materials to be described. This extensions includes both materials that are essentially single phase but with coarse inclusions, and materials that have a large volume fraction of a second phase.

4:30 PM

Delineation of the Mechanical Performance Closures for Polycrystalline fcc Metals Using First-Order Homogenization Theories: *Gwenaelle Proust*[1]; Surya R. Kalidindi[1]; [1]Drexel University, MSE, 3100 Market St., Philadelphia, PA 19104 USA

The mechanical properties and performance of a given material depend on its microstructure, which includes several aspects such as the chemical composition, the average grain size and the crystallographic texture. Of these, crystallographic texture is perhaps the most dominant microstructural feature that controls the elastic-initial yield properties of polycrystalline metals used in manufacture of most engineering components. Using a spectral representation of the texture and its relationship with the overall elastic-initial yield properties of materials, we are able to delineate the complete property closure for polycrystalline cubic materials. This property closure describes the full range of feasible elastic-plastic properties for a given material system. First order homogenization theories based on the Hill-Paul bound theorems have been used for the elastic properties, while the Sachs and Taylor models have been used to define the bounding estimates on the plastic yield properties. The proposed methodology has been used successfully to develop a few examples of property closures for classic design problems in mechanical engineering, such as those encountered in design of compliant mechanisms and elastic hinges. On the performance closures, we have also identified the locations of readily available or easily processable textures such as rolled textures, drawn textures, and cube textures, thereby providing valuable guidance to the designers in selection of materials.

Advancements in Mechanical Property Characterization at the Micro- and Nano-Scale: Application of Nanoindentation Methods

Sponsored by: TMS - Structural Materials Division
Program Organizers: Mike Uchic, Air Force Research Laboratory, Dayton, OH 45433-7817 USA; Kevin J. Hemker, Johns Hopkins University, Department of Mechanical Engineering, Baltimore, MD 21218 USA; Marc Zupan, University of Maryland, Baltimore, MD 21250 USA

Wednesday PM — Room: Mardi Gras Ballroom B
September 29, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Marc Zupan, Univeristy of Maryland, Dept. of Mechl. Engrg., Baltimore, MD 21250 USA; Michael Uchic, Air Force Research Laboratory, Matls. & Mfg. Direct., Wright Patterson AFB, OH 45459 USA

2:00 PM

Estimation of Single-Crystal Elastic-Plastic Properties Using Nano-Indentation, Orientation Imaging Microscopy and Finite Element Simulations: *Gwenaelle Proust*[1]; Surya R. Kalidindi[1]; [1]Drexel University, MSE, 3100 Market St., Philadelphia, PA 19104 USA

Nano-indentation is being widely used as a technique to estimate the Young modulus and the hardness of materials. In this study we will show that by measuring the crystal orientation of the grain at the indentation site using orientation imaging microscopy (OIM) and simulating the load-displacement curves obtained during nano-indentation experiments with finite element modeling, it is possible to extract the basic single crystal elastic and plastic properties of polycrystalline materials. Our methodology explicitly accounts for the inherent anisotropy in the material at the single crystal level. The proposed methodology has been successfully applied to pure aluminum and pure titanium. The advantages and limitations of the proposed methodology are discussed in this detail in this paper. In general, the use of finite element methods for extracting the modulus of the sample from the measured load-displacement curve, in place of the analytical methods being used in current literature, provided significantly better results.

2:20 PM

Nanoindentation of Platinum at Elevated Temperatures: *Andrea Maria Hodge*[1]; Alan C. Lund[2]; Christopher A. Schuh[2]; [1]Lawrence Livermore National Laboratory, Chmst. & Matls. Sci., PO Box 808, L-350, Livermore, CA 94550 USA; [2]Massachusetts Institute of Technology, 77 Mass. Ave., Cambridge, MA 02139 USA

The onset of plastic deformation during nanoindentation is studied, focusing upon the effects of temperature variation. By performing indentations on pure (100), (110) and (111)-oriented platinum at room temperature, 100 and 200° C, we demonstrate that higher temperatures promote the discretization of plasticity into sharp bursts of activity. We also will discuss the transition from elastic to plastic deformation as temperature is increased and as a function of orientation. Current results are in line with expectations for stress-biased, thermally-activated deformation processes.

2:40 PM

Nanoscale Toughening Secrets of Natural Seashell Nanocomposites: *Xiaodong Li*[1]; Patrick Nardi[1]; Wei-Che Chang[1]; Yuh J. Chao[1]; Rizhi Wang[2]; Ming Chang[3]; [1]University of South Carolina, Dept. of Mechl. Engrg., 300 Main St., Columbia, SC 29208 USA; [2]University of British Columbia, Dept. of Metals & Matls. Engrg., 309 - 6350 Stores Rd., Vancouver, BC V6T 1Z4 Canada; [3]Chung Yuan Christian University, Dept. of Mechl. Engrg., 22 Pu-Jen, Pu-Chung Li, Chung-Li (32023), Taiwan China

Nature has evolved highly complex and elegant mechanisms for materials design and synthesis. Living organisms produce materials with physical properties that still surpass those of analogous synthetic materials with similar phase compositions. Nature has long been using bottom-up nanofabrication method to form self-assembled nanomaterials that are much stronger and tougher than many man-made materials formed top-down. Nanoscale structural and mechanical characterization of the shells of Pectinidae and red abalone has been carried out. Hardness and elastic modulus were measured by nanoindentation using a nanoindenter. Micro/nanoscale cracks were generated by microindentation using a microindenter. The shell surface structure, crossed lamellar structure, and indentation cracks were imaged using an optical microscope, an atomic force microscope (AFM) and a scanning electron microscope (SEM). Fracture mechanisms were discussed in conjunction of its architecture, hardness, elastic modulus, and energy-dissipation during cracking.

3:00 PM
Mechanical Characterisation of Fe(Cr)-Si-B Metallic Glass Wire by Ultra Micro Indentation: *Ayodele Oladimeji Olofinjana*[1]; Rai Indra Wardana[2]; [1]Universiti Brunei Darussalam, Faculty of Sci., Tungku Link Brunei; [2]Queensland University of Technology, Brisbane Australia

Metallic glass wire products are known for their additional high static and fatigue strength. The thermodynamic and kinetic requirements for the formation of amorphous structures in readily glass forming alloys require rapid solidifications of the order of 106K per second. This rapid cooling rate requirement imposes a theoretical section thickness of less than 200mm diameter for glassy metallic wires. In practice, metallic glass wires are more commonly cast as 100mm diameter. This unusual dimension presents difficulty for the use of traditional methods for the mechanical characterisation of the high strength these metallic glass wires. The advent of ultra- and nano- indentation techniques provides a new way of easily measuring the mechanical properties of high strength thin-sectioned bodies. In this work, we report the use of Ultra-micro indentation system (UMIS 2000) to characterise the mechanical properties of Fe(Cr)SiB metallic glass wires. The analysis of the load displacement data allowed us to use indentation mechanics for the elastic contact and from which we can determine a representative a stress-strain curve. This new representative stress-strain relationship can give an indication of the plastic properties, which are not as clear in conventional pull type tensometer tests. The elastic modulus observed for the wire varied from 150-160GPa. The hardness and representative strength determined from the indentation tests were respectively of the order of 1000Hv and 4000MPa.

3:20 PM Break

3:40 PM
Micro/Nanomechanical and Tribological Characterization of Orthopedic Materials: *Xiaodong Li*[1]; Xinnan Wang[1]; Tangali S. Sudarshan[2]; Yuehei H. An[3]; Julie Morris[2]; Natarajan Sethuraman[4]; [1]University of South Carolina, Dept. of Mechl. Engrg., 300 Main St., Columbia, SC 29208 USA; [2]University of South Carolina, Dept. of Electl. Engrg., 300 Main St., Columbia, SC 29208 USA; [3]Medical University of South Carolina, Orthopedic Rsch. Lab., 96 Jonathan Lucas St., CSB708, Charleston, SC 29425 USA; [4]GlycoFi, Inc., 21 Lafayette St., Ste. 200, Lebanon, NH 03766 USA

Mechanical and tribological aspects are of critical importance in determining long-term stability of medical implants and devices. Aseptic loosening of total joint replacements begins as a mechanical problem, which is initiated by joint articulation and other relative motion between surfaces. Wear debris can cause calcar resorption and implant loosening. An in-depth understanding of the mechanical and tribological properties of biomaterials is therefore fundamental to the control of fracture failure and wear in new implants. Micro/nanomechanical and tribological characterization of SiC, CoCrMo, Ti-6Al-4V, and stainless steel was carried out using a nanoindenter and a microtribometer. Micro/nanoscale deformation and fracture mechanism were studied in conjunction with hardness, elastic modulus, scratch and wear resistance. SiC exhibits the highest hardness and elastic modulus as well as the lowest scratch and wear resistance compared with other currently used orthopedic materials, and should find more applications in the field of bioengineering.

4:00 PM
Nano-Mechanical Testing for Fracture of Oxide Films: *K. R. Morasch*[1]; [1]Washington State University, Mechl. & Matls. Engrg., PO Box 642920, Pullman, WA 99164-2920 USA

Nanoindentation was used to test the mechanical properties of aluminum oxide grown on an aluminum substrate. The oxides were thermally grown for 1, 2, and 3 hrs at 500C. The ultimate strength of the oxide was determined for varying oxide thicknesses. Indentations into these oxides exhibit plastic deformation at loads below a yield and fracture excursion. This indicates that the excursion was caused by oxide fracture and not the initiation of yielding in the substrate. The load at which film fracture occurred was independent of oxide thicknesses, but the indenter penetration depth was not. The ultimate strength of the oxide was found using an analytical model, and increased as the film thickness increased. The oxide film thicknesses were 8, 12, and 49 nm, which results in ultimate strengths of 1.2, 1.9, and 6.5 GPa, respectively. Underlying grain orientation does not impact the strength of the oxide film.

4:20 PM
Synthesis and Mechanical Characterization of Nanocrystalline Al-Pb Alloys: *Koteswararao V. Rajulapati*[1]; Ronald O. Scattergood[1]; K. Linga Murty[1]; Carl C. Koch[1]; [1]North Carolina State University, Dept. of Matls. Sci. & Engrg., 229, Riddick, Stinson Dr., Raleigh, NC 27695-7907 USA

Nanocrystalline aluminum-lead (Al-Pb) alloys were synthesized by high energy ball milling at room temperature. Lead particles are dispersed through out the aluminum matrix as second phase. Here the crystallite sizes of both the matrix and the second phase are in the nano regime. The powder samples are subsequently hot compacted under uniaxial loading conditions in an argon atmosphere. The structural characterization was done by x-ray diffraction (XRD) and transmission electron microscopy (TEM). The mechanical properties are evaluated by micro hardness measurements and several small specimen mechanical testing procedures. In this paper, the evolution of microstructure and mechanical behavior of different nanocrystalline Al-Pb alloys will be discussed. (This research is supported by the US National Science Foundation under grant number DMR 0201474).

4:40 PM
Nanoscale Structural and Mechanical Studies of Single-Wall Carbon Nanotube-Reinforced Epoxy Composites: *Xiaodong Li*[1]; Hongsheng Gao[1]; Wally A. Scrivens[2]; Dongling Fei[2]; Xiaoyou Xu[2]; Michael A. Sutton[1]; Anthony P. Reynolds[1]; Michael L. Myrick[2]; [1]University of South Carolina, Dept. of Mechl. Engrg., 300 Main St., Columbia, SC 29208 USA; [2]University of South Carolina, Dept. of Mechl. Engrg., 631 Sumter St., Columbia, SC 29208 USA

Exceptional physical properties, high aspect ratio and low density of single wall carbon nanotubes (SWNTs) have made them ideal candidates for developing the next generation of SWNT/polymer composites. In this study, the hardness and elastic modulus of SWNT reinforced epoxy composites were measured using a nanoindenter. Scratch resistance and scratch damage were studied using the AFM tip sliding against the SWNT reinforced sample surfaces. Nanoindentation/nanoscratch deformation and fracture behavior was studied by in-situ imaging of the indentation impressions/scratch tracks. Viscoelastic properties of the composites were measured using nanoindentation dynamic mechanical analysis tests. The present nanoscale mechanical research results present additional insight on the understanding of dispersion, interfacial bonding, and load transferring mechanisms at work in the SWNT reinforced polymer composites.

5:00 PM
TEM Investigation of INCONEL 740 and Modified INCONEL 740 as Candidate Materials for Ultrasupercritical (USC) Coal Power Plants: *Quanyan Wu*[1]; John Shingledecker[2]; Vijay Vasudevan[1]; Robert W. Swindeman[2]; [1]University of Cincinnati, Chem. & Matls. Engrg., 2624 Clifton Ave., Cincinnati, OH 45220 USA; [2]Oak Ridge National Laboratory, Ceram. & Metals, Bldg. 4500S, MS6155, PO Box 2008, Oak Ridge, TN 37831 USA

New alloys have been developed to meet higher temperature demands for higher thermal efficiency and lower CO_2 release in coal power plants. Inconel 740 is a new nickel-base superalloy which has shown good thermal stability and strength to 750°C. The major precipitates were MC, $M_{23}C_6$ and gamma prime when solutionized at 1050°C. Large amounts of eta precipitates formed a Widmanstätten pattern when creep-tested at 816°C and 138MPa for 319.9 hours, in addition to gamma prime rafting. Modified IN740 showed reduction of eta phases and better creep strength. Aging of both modified and unmodified Inconel 740 were carried out at different temperatures, up to 500 hours to observe microstructural development, using OM, EDS, SEM and TEM. In particular, the orientation, structure, distributions and morphology of phases (including gamma, gamma prime,eta, carbides, etc) were emphasized. Microhardness is measured as an indication of the associated mechanical properties.

Applications of Orientation Microscopy Techniques to Phase Transformations: Nonferrous Alloys

Sponsored by: TMS - Materials Processing & Manufacturing Division, TMS - MPMD-Phase Transformations Committee-(Jt. ASM-MSCTS)
Program Organizers: Robert E. Hackenberg, Los Alamos National Laboratory, Materials Science and Technology Division, Los Alamos, NM 87545 USA; Richard W. Fonda, Naval Research Laboratory, Washington, DC 20375 USA; Milo V. Kral, University of Canterbury, Department of Mechanical Engineering, Christchurch New Zealand

Wednesday PM — Room: Mardi Gras Ballroom C
September 29, 2004 — Location: Marriott New Orleans Hotel

Session Chair: Cesar J. Buque, GKSS Rsch. Ctr., Inst. for Matls. Rsch., Geesthacht 21502 Germany

2:00 PM Invited
EBSD and EDX Studies of the Microstructural Features Occurring in the Interdiffusion Zone of Diffusion Bonded Gamma-TiAl-Based Alloys: *Cesar Justino Buque*[1]; Stefan Eggert[1]; Fritz Appel[1]; [1]GKSS Research Centre, Inst. for Matls. Rsch., Max-Planck-Str. 1, Geesthacht 21502 Germany

The microstructural modifications occurring during diffusion bonding of two phase $Ti_3Al(\alpha_2)/TiAl(\gamma)$ titanium aluminide alloys were investigated. Cylindrical specimens were bonded under vacuum at 1220 K and a pressure of 60 MPa applied for 2 hours. The study involves energy dispersive X-Ray (EDX) for chemical analysis and electron back-scattered diffraction (EBSD) for phase identification and texture analysis. The combination of SEM, EDX and EBSD gives the opportunity to explore the micromechanisms of diffusion, phase transformations and recrystallization involved in diffusion bonding. After diffusion bonding, α_2 grains surrounded by equiaxed γ grains were homogeneously formed at the interdiffusion zone. The formation of this interdiffusion layer is probably driven by the unavoidable contamination of the diffusion couple with oxygen, which is known to stabilize the α_2 phase. The structural details on the newly formed granular microstructures depend on alloy composition and phase constitution. In general, a strong {1 0 -1 0}-texture parallel to the direction of the bonding force developed in the (α_2 phase revealing that the nucleation process of the α_2 grains occurs preferentially in such a way that the corresponding crystal lattice can deform by prismatic glide. The EDX analysis revealed that the α_2 grains formed at the interdiffusion zone are rich in Al. Thus, there is a high density of Al anti-site defects, i.e., Al atoms situating on the Ti-sublattice in the newly formed α_2 phase. The antisite defects probably support the diffusion process that is needed to accomplish the structural changes observed in the diffusion zone.

2:30 PM
The Effect of the Differences in the Starting Microstructure in an Alpha/Beta Ti Alloy on the Microtexture of the Globular Alpha Formed by the Hot Compression of Such Alloys: *Dhriti Bhattacharyya*[1]; Gopal Viswanathan[1]; Sujoy Kar[1]; Hamish L. Fraser[1]; [1]Ohio State University, Matls. Sci. & Engrg., 477 Watts Hall, 2041 College Rd., Columbus, OH 43201 USA

The microtexture of globular alpha in two phase alpha/beta Ti alloys is of significant importance to their mechanical properties. Hot working of beta transformed microstructures, a prerequisite processing step for globularization of alpha laths, determines the characteristics such as size, distribution and microtexture of globular alpha in the microstructure. It has been suggested that globularization occurs by the penetration of beta into the small angle grain boundaries between recrystallized segments of alpha laths, or at the shear bands in alpha laths. This study aims to show that for the alpha/beta Ti alloy studied, i.e. Ti-6Al-2Sn-4Zr-6Mo, the nature and characteristics of the globular alpha microtexture significantly depends on the starting microstructure prior to the hot working process. Extensive Orientation Imaging Microscopy (OIM) was done to demonstrate this phenomenon. The microtexture results will be presented and a possible explanation for globular alpha microtexture shall be forwarded.

2:55 PM
The Phase Transformation Behavior and Grain Boundary Character Distribution in Ti-Al-Nb Alloys: *Dingqiang Li*[1]; Carl J. Boehlert[1]; [1]Alfred University, Sch. of Engrg., 2 Pine St., Alfred, NY 14802 USA

The phase transformation behavior and grain boundary character distribution (GBCD) of Ti-Al-Nb alloys containing the hexagonal (α_2), body-centered-cubic (BCC) and orthorhombic (O) phases were investigated. The alloys, which ranged in composition between 12-26at.%Al and 25-38at.%Nb, were prepared by induction melting or processed by pancake forging and hot-packed rolling. Using electron backscatter diffraction (EBSD), the twin-related O-phase variant interfacial planes, most likely formed from α_2-to-O transformation, were identified and quantified following pancake forging and hot rolling. The {110} boundary plane twin variants, characterized by an approximately 64.4° rotation about [001], represented up to 28% of the O-phase boundaries, while up to 5% of the O boundaries exhibited {130} planes and were associated with an approximately 54.6° rotation about [001]. Thus, EBSD analysis proved to be a useful technique for determining the fraction of O-variant plane boundaries and distinguishing variant selection. For the induction melted alloy, the BCC-O transformation was characterized using EBSD and XRD and it was found that the O variants formed in a fine lath network within the parent BCC. An approximately equal distribution of the 6 resolvable O variants were formed from this transformation. Thus, no variant dominated nucleation and/or growth events during the slow transformation from the parent BCC and subsequent cooling. This work was supported by NSF Grant DMR-0134789.

3:20 PM Break

3:40 PM
Characterization of Casting Defects in Ni-Base Superalloys Using Various Electron Microscopy Techniques: *Erik M. Mueller*[1]; Kevin E. Kloske[2]; Michael J. Kaufman[3]; Vladi Levit[4]; [1]University of Florida, Matls. Sci. & Engrg., 131 Rhines Hall, Gainesville, FL 32611 USA; [2]Pratt & Whitney, Matls. & Process Engrg., Aircraft Rd., M/S 403-35, Middletown, CT 06457 USA; [3]University of North Texas, Dept. of Matls. Sci. & Engrg., PO Box 305310, Denton, TX 76203-5310 USA; [4]Gas Turbine Materials Associates, 401 Isom Rd., Ste. 470, San Antonio, TX 78216 USA

In directionally solidified and single crystal castings of Ni-base superalloys, casting defects such as freckles and scale occasionally form and lead to rejection of parts causing a substantial decrease in production efficiency. Several different approaches have been used to prevent these defects, which entail modifying compositions and/or adjusting processing conditions. In this study, castings of CMSX-4 and PWA-1483 with scale and castings of nominal René N4 and PWA 1483 with freckle chains were analyzed using TEM, SEM, EBSD, and EDS/WDS. It will be shown that the mechanism of scale formation involves solute-rich interdendritic liquid being exuded into the gap between the casting surface and the mold and reacting with the mold material. The nature of this interaction depends on the compositions of the alloy and the mold, and it produces a range of undesirable phases at the casting surface. The freckles, on the other hand, are the result of thermosolutal convection in the mushy zone during solidification. The orientation of the freckle grains and the scale was determined using EBSD and found to be independent of the adjacent crystal orientation. The implications of these observations will be discussed in light of current casting practices.

4:05 PM
Identification of Intermetallic Phases in Al-Si Alloys Using EBSD: *Milo V. Kral*[1]; [1]University of Canterbury, Mechl. Engrg., PO Box 4800, Ilam, Christchurch New Zealand

Iron-rich intermetallic phases are well known to be strongly influential on mechanical properties in cast eutectic Al-Si alloys. Two important phases have been previously designated as the relatively benign alpha-phase (with a "Chinese Script" morphology) and the detrimental beta-phase (plate or needle-shaped). While the morphologies and effects of these phases are generally agreed upon, there is no agreement in the literature regarding the chemistry or crystallography of these phases. In the present work, various intermetallic phases in cast eutectic Al-Si alloys were characterized using a combination of scanning electron microscopy, energy dispersive x-ray spectroscopy and electron backscatter diffraction pattern analysis. The alpha-phase particles were consistent with cubic Al19Fe4MnSi2 and beta-phase particles were most consistent with tetragonal Al3FeSi2.

4:30 PM
Intermetallic Phase Analysis in Aluminium Alloys: *Soonwuk Cheong*[1]; [1]Alcoa, Inc., Matls. Sci., 100 Tech. Dr., Alcoa Ctr., PA 15206 USA

A range of different alloying additions are added to aluminium castings depending on the final application. Homogenization of the aluminium cast reduces segregation and promotes the transformation of metastable secondary and ternary phases into equilibrium phases, resulting in precipitation of dispersoids in certain cases. The identity, size and distribution of the secondary and ternary intermetallic have critical importance on the material properties of the alloy. In the present study, the crystallography and morphology of the secondary and ternary phases in Aluminium alloys are examined with EBSD and EDS analyses under thermodynamic considerations.

Materials and Critical Societal Issues Special Session

Sponsored by: TMS, TMS - Public & Governmental Affairs Committee, ASM International Federal Affairs Committee
Program Organizer: Diran Apelian, Worcester Polytechnic Institute, Metal Processing Institute, Worcester, MA 01609-2280 USA

Wednesday PM — Room: La Galerie 1
September 29, 2004 — Location: Marriott New Orleans Hotel

Session Chair: Diran Apelian, Worcester Polytechnic Institute, Metal Procg. Dept., Worcester, MA 01609 USA

2:00 PM Opening Remarks by Diran Apelian

2:10 PM Invited
The Food Industry's Global Challenges and Opportunities: *Beat Haeni*[1]; [1]Buhler Group, Uzwil Switzerland

Food and eating habits are closely related to the technologies available to produce and distribute foods. They have developed from just "looking for sources" to today's objectives to get a "complete balanced nutrition". The information about structure and content of food products and especially the deeper insight in the digestion process has opened new possibilities of designed foods. This results in the new trends such as low-carb foods, whole wheat or fiber enriched foods.

2:45 PM Invited
Materials in Architecture: Will We Ever Meet the Demands?: *Spiro N. Pollalis*[1]; [1]Harvard Design School, Design Tech. & Mgmt., Ctr. for Design Informatics, Cambridge, MA USA

In architecture, we ask for the impossible: extraordinary properties of structural materials and immortality of the construction materials, at a low cost and with a long performance warranty. We also ask for a new generation of materials, integrated with sensors, with changing properties subject to changing conditions, with built-in logic. Yet, today, architecture bases the thrust of its innovation on creating form and space, introducing new assemblies and uses of centuries-old materials. With no central authority to institute changes in the highly fragmented design and construction industry, this presentation focuses on the needs of architects, such as continuous performance with no-down time, and handling the sun, the rain and temperature cycles, with affordability and sensitivity to the environment. Case studies demonstrate such requirements, the adopted solutions, and their compromises and opportunities with today's available materials. Then, new demands are examined, springing from applications of information technology integrated into material properties and thoughts about future developments.

3:20 PM Break

3:35 PM Invited
Recycling Opportunities, Technical Challenges, and Illusions: *David B. Spencer*[1]; [1]wTe®Corporation, Bedford, MA USA

David Spencer has played an industry leadership role in recycling of municipal solid waste, plastics, glass, paper, and metals for over 35- years. He has hands-on operating experience with numerous recycling projects ranging in size from a small curbside collection program in his hometown of Bedford, Massachusetts to a $100 Million plus facility for recycling 1000 tons per day of municipal solid waste and 350 tons per day of sewage sludge in Wilmington, Delaware. Currently, he is CEO of wTe®Corporation which owns and operates various recycling facilities for metals and plastics: one of which is wTe Recycling, Inc. — one of New England's three major automobile shredder operations, and another of which is UltrePET® LLC — the 3rd largest plastics recycler in the U.S. processing millions of PET soda bottles per day. His latest activities involve high-speed opto-electronic sorting of metals by alloy type at high speed. He will provide a business and technology perspective on recycling, particularly recycling of household waste, metals and plastics.

4:10 PM Invited
Restoring Health, from Replacement Parts to Regenerative Medicine: Challenges and Opportunities: *Arthur J. Coury*[1]; [1]Genzyme Corporation, Cambridge, MA USA

The development of modern materials such as structural polymers and metal alloys enabled the implementation of many medical therapeutic devices and drug delivery systems over the past half century. These biomaterials-based products, which often served to replace the function of organs, included devices such as prosthetic joints, teeth, lens, valves, breasts, pacemakers and bones. In the present era, the focus of medicine has shifted and the knowledge we have gained in physiology, cellular and molecular biology provides the potential for supplanting many mechanical, chemical and electronics-based therapies by inducing the body to heal and regenerate its structures and functions. As with many disruptive technologies, regenerative medicine approaches such as those found in tissue engineering, gene therapy and growth factor implementation have experienced early resistance and setbacks. But the concepts are valid, major successes are unfolding and the era of regenerative medicine is arriving with only the timing in question. To achieve these breakthroughs, advanced materials technologies will be required to deliver, augment or enable the cellular and molecular components of regenerative medicine.

4:45 PM Invited
Trends in Vehicle Resource Consumption: *Randolph Kirchain*[1]; [1]Massachusetts Institute of Technology, Dept. of Matls. Sci. & Engrg. & Engrg. Sys. Div., Cambridge, MA 02139 USA

Although the definition and execution of global sustainability is still debated, a significant element will certainly be the effective management of material resources. The automotive industry – a major consumer across numerous metal and non-metal markets - will play a significant role. Furthermore, the growth of the world automotive fleet in developing and transitional nations will ensure that this consumption prominence will remain strong. Given that context it is illustrative to understand how current vehicle trends will affect the consumption of major engineering materials. The talk will examine several scenarios of emergent vehicle technology penetration including both material and propulsion changes. The implications of these shifts on primary consumption and secondary supply will be discussed. Results from related studies on the evolution of fuel use and fossil resource consumption will be compared.

Materials Damage Prognosis: Materials Failure and Signature Analysis

Sponsored by: TMS - Structural Materials Division
Program Organizers: James M. Larsen, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson AFB, OH 45433-7817 USA; Jeffrey R. Calcaterra, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson Air Force Base, OH 45433-7817 USA; Leo Christodoulou, Defense Advanced Research Agency, Arlington, VA 22203-1714 USA; Michael L. Dent, Anteon Corporation USA; William J. Hardman, Naval Air Systems Command, Propulsion and Power Directorate (AIR 4.4.2), Patuxent River, MD 20670-1534 USA; Paul Hoffman, United States Navy, NAVAIR, Patuxent River, MD 20670 USA; J. Wayne Jones, University of Michigan, College of Engineering, Department of Materials, Science and Engineering, Ann Arbor, MI 48109 USA; Stephan M. Russ, Air Force Research Laboratory, Materials and Manufacturing Directorate, AFRL/MLLN, Wright-Patterson Air Force Base, OH 45433-7817 USA

Wednesday PM Room: La Galerie 6
September 29, 2004 Location: Marriott New Orleans Hotel

Session Chairs: William J. Hardman, NAVAIR, Patuxent River, MD 20670-1534 USA; James Malas, Air Force Research Laboratory, Wright Patterson AFB, OH 45433 USA

2:00 PM
ProDAPS: Intelligent Tools for Materials Damage Prognosis: *Brian David Larder*[1]; Rob Callan[1]; [1]Smiths Aerospace, Elect. Sys. - Southampton, School Ln., Chandlers Ford, Eastleigh, Hampshire SO53 4YG UK

Although there is much emphasis on the development of new sensor technologies for the local interrogation of materials damage state, the cost and difficulties associated with adding sensors to components in complex mechanical systems means that global methods and sensors have an important role in materials prognostics. ProDAPS (a Probabilistic Diagnostic and Prognostic System), which is being developed on an AFRL DUS&T program, provides an integrated suite of intelligent tools aimed at enhancing global methods for materials damage prognosis. The ProDAPS intelligent tools for data mining, knowledge discovery, data fusion and reasoning are essential for complex mechanical systems where physics-based models will be subject to practical limitations. ProDAPS' contribution to material damage prognostics will be explored through an analysis of its capabilities within two different global sensor applications. These are the performance monitoring of in-service gas turbine engines, and the vibration health monitoring of in-service helicopter drive trains.

2:25 PM
Prediction of Crack Paths Based Upon Detailed Microstructure Characterization in a Near-g TiAl Alloy: *Boon-Chai Ng*[1]; Tom R. Bieler[1]; Martin A. Crimp[1]; [1]Michigan State University, Chem. Engrg. & Matls. Sci., E. Lansing, MI 48824 USA

Fracture in a duplex g-TiAl alloy with equiaxed grains has been studied. The crack path in a notched Mode I crack growth specimen was analyzed using a combination of orientation imaging microscopy and selected angle channeling patterns (to obtain the true c-axis orientation in each grain). A phenomenological fracture initiation parameter incorporating the contributions from deformation twinning and ordinary dislocation systems has been developed, that is capable of identifying boundaries that are likely to nucleate microcracks. This fracture initiation parameter was then used to analyze the existing crack path to explain why sharp turns in the crack path occurred. With this understanding, grain boundaries in the microstructure ahead of the crack tip were analyzed to predict the expected fracture path, and to compare it to the actual crack path. Based upon this parameter, criteria for crystal orientations and misorientations for high toughness microstructures are proposed. Supported by AFOSR F49620-01-1-0116.

2:50 PM
Prediction of the Relationship Between Microstructure and Fatigue Damage for a Turbine Disk Alloy by Ultrasonic Techniques: *A. Shyam*[1]; C. J. Torbet[1]; S. K. Jha[2]; J. M. Larsen[3]; M. J. Caton[3]; C. J. Szczepanski[1]; T. M. Pollock[1]; J. W. Jones[1]; [1]University of Michigan, Matls. Sci. & Engrg., 3062 H H Dow, Ann Arbor, MI 48197 USA; [2]Universal Technology Corporation, Dayton, OH 45432 USA; [3]AFRL/MLLMN Wright Patterson AFB, Matls. & Mfg. Direct., Dayton, OH 45433 USA

Understanding the relationship between fatigue damage and the underlying microstructure is of paramount importance to predict the response of a turbine disk alloy under service conditions. The recent development of ultrasonic fatigue techniques allows rapid determination of microstructural neighborhoods which are responsible for initiation of fatigue damage. An ultrasonic fatigue testing system capable of testing at temperatures as high as 800°C and at positive mean stresses will be described. Results for the characterization of ultrasonic (20 kHz) fatigue behavior of the nickel-base superalloy Rene' 88 DT in the lifetime regime of 105 to 109 at 20 and 593°C with a stress-ratio of 0.05 will be presented. The crack initiation sites in this alloy were favorably oriented large grains and inclusions. Small crack growth behavior obtained by initiating cracks from micronotches machined with femtosecond pulsed lasers is compared at both conventional and ultrasonic frequencies. The size range of these notches is in the range of grain and inclusion size in this superalloy. A probabilistic model incorporating crack initiation, small and long crack propagation regimes of total life would be presented.

3:15 PM Break

3:25 PM Invited
Early Stage Fatigue Damage Detection and Characterization for Prognostics Model Validation: *Neil Goldfine*[1]; Vladimir Zilberstein[1]; Chris Craven[1]; David Grundy[1]; Robert Silberstein[2]; Steven Chu[2]; [1]JENTEK Sensors Inc., 110-1 Clematis Ave., Waltham, MA 02453-7013 USA; [2]Northrop Grumman, AEW/EW

This paper describes the use of surface mounted MWM-Array eddy current sensors for early stage damage detection in fatigue coupons. Specifically, the electrical conductivity and lift-off changes associated with surface roughening are monitored. Capability is demonstrated for detection of small changes associated with early stage fatigue damage. The focus of this effort is to provide model validation for fatigue damage models being developed under the DARPA funded Northrop Grumman Structural Integrity Prognosis System (SIPS) program. This paper describes coupon test results with sensors mounted inside holes in aluminum alloy coupons. Scanning electron microscopy results are also provided to validate detections and to assess capability. In addition, new methods for detection of cracks under fastener heads using segmented field MWM-Arrays are described. These sensors use multiple sensing elements at varied positions relative to the drive winding to enable removal of fastener interference effects and reveal the presence of small cracks under fasteners. This new capability offers the potential to detect relatively small buried cracks, e.g., under fastener heads, using sensors mounted on accessible surfaces.

3:50 PM Invited
Adaptive Prognosis Applied to Corrosion/Fatigue: *David S. Muench*[1]; Gregory Kacprzynski[1]; Michael J. Roemer[1]; Robert Wei[2]; Gary Harlow[2]; [1]Impact Technologies, LLC, 125 Tech Park Dr., Rochester, NY 14623 USA; [2]Lehigh University, Dept. of Mechl. Engrg., 7 Asa Dr., Bethlehem, PA 18015 USA

Corrosion initiated fatigue cracks can be a significant failure mode for aging aircraft structures. Sophisticated corrosion/fatigue models exist that can predict failure progression in laboratory environments with controlled materials, usage profiles and environmental conditions. The prognostic challenge however, is to accurately employ such models in the field where a priori factors and loading are far less certain and damage state awareness much more imprecise. As a test case for addressing this challenge, an adaptive corrosion/fatigue module was developed under DARPA's Structural Integrity Prognosis System (SIPS) that fuses model-based prognosis with various imperfect sources of both continuous and discontinuous data in an attempt to improve the accuracy of Remaining Useful Life (RUL) predictions. Specifically, a corrosion/fatigue growth model developed by Wei and Harlow of Lehigh University is introduced and demonstrated via internal variable updates and the application of a Kalman filter to properly fuse available model and sensor information. Corrosion/fatigue model transition criteria are addressed stochastically and RUL prediction results are presented with and without adaptation in the context of potential operational and maintenance (O&M) decisions.

4:15 PM
Models for Ductile Failure Applied to Anisotropic Al2024-T351: *Dirk Steglich*[1]; Davide Paganelli[1]; Thomas Pardoen[2]; [1]GKSS Research Center, WMS, Max-Planck-Str. 1, Geesthacht 21502 Germany; [2]Université catholique de Louvain, Louvain-la-Neuve 1348 Belgium

Al2024—T351 is an aluminium alloy renowned for its good mechanical properties, its light weight characteristics and its resistance to corrosion. Therefore it is used since decades in thin rolled sheets for aircraft applications. For machined components, the mechanical properties in the thickness direction become additionally relevant. While the yielding behaviour is found to be almost isotropic, ductility in thickness direction is less than in rolling direction. Thus it is important to account for anisotropy in damage behaviour. Damage models accounting for the void shape and distribution might be able to fulfill this task. In the following work, a Gologanu-type model will be applied and compared with unit cell calculations as well as with results of the isotropic Gurson model including Thomasons coalescence criterion. The predictions will be compared with test results of Al2024-T351-specimens.

4:40 PM
Damage Evolution in Fatigue of a Nickel-Base Superalloy and its Effect on the Variability in Life: *Sushant K. Jha*[1]; Michael J. Caton[2]; James M. Larsen[2]; Andrew H. Rosenberger[2]; [1]Universal Technology Corp., 1270 N. Fairfield Rd., Dayton, OH 45432 USA; [2]Air Force Research Laboratory, AFRL/MLLMN, 2230, 10th St., Ste. 1, Wright Patterson AFB, OH 45433 USA

One of the primary themes of the materials damage prognosis approach is to base life management on real-time information of evolving damage. Combining the awareness of damage with probabilistic life prediction can significantly reduce the uncertainty in lifetimes. In light of this, the paper examines the factors controlling the variability in fatigue life of a turbine disk superalloy, Rene '88 DT. Specifically, the role of damage evolution at the microscopic size scale and the subsequent crack initiation and growth regimes in causing the uncertainty in lives will be discussed. Due to the dependency of slip characteristics on temperature and strain rate (i.e., frequency), study of fatigue behavior with respect to these variables provided an understanding of the operating deformation mechanisms. A life prediction model based on the distribution in the degree of deformation accumulation as controlled by the variation in the local microstructure will also be discussed.

Mechanical Behavior of Body-Centered-Cubic (BCC) Metals and Alloys: Texture, Radiation, and Solute Effects

Sponsored by: TMS - Structural Materials Division, TMS - SMD-Mechanical Behavior of Materials-(Jt. ASM-MSCTS), TMS - SMD-Refractory Metals Committee, TMS - SMD-Structural Materials Committee
Program Organizers: George T. Gray III, Los Alamos National Laboratory, Dynamic Properties Team, Los Alamos, NM 87545-0001 USA; Thomas R. Bieler, Michigan State University, Department of Chemical Engineering and Materials Science, East Lansing, MI 48824-1226 USA; John J. Lewandowski, Case Western Reserve University, Department of Materials Science and Engineering, Cleveland, OH 44106 USA; Eric M. Taleff, University of Texas, Mechanical Engineering Department, Austin, TX 78712-1063 USA

Wednesday PM   Room: Mardi Gras Ballroom A
September 29, 2004   Location: Marriott New Orleans Hotel

Session Chairs: Thomas R. Bieler, Michigan State University, Matls. Sci. & Mech., E. Lansing, MI 48824-1226 USA; George (Rusty) T. Gray III, Los Alamos National Laboratory, Matls. Sci., Los Alamos, NM 87545-0001 USA

2:00 PM
Effect of Rolling and Annealing Parameters on Recrystallization of Cold Rolled High Purity Niobium: *Hairong Jiang*[1]; *Thomas R. Bieler*[1]; Chris Compton[2]; Terry L. Grimm[2]; [1]Michigan State University, Chem. Engrg. & Matls. Sci., 2527 Engrg. Bldg., E. Lansing, MI 48824-1226 USA; [2]Michigan State University, Natl. Superconducting Cyclotron Lab., East Lansing, MI 48824 USA

The development of the cold rolling and recrystallization textures in high purity niobium was investigated for various rolling and annealing parameters. Texture was characterized using x-ray diffraction and orientation imaging microscopy, to obtain the orientation distribution function (ODF). Gradients in the microstucture and texture from surface to interior are strongly dependent on the rolling parameters and history of rolling process. Unlike steels, the texture after annealing remains nearly unchanged after recrystallization. Since the elastic behavior in Nb and Fe are opposite (stiffest directions in Fe <111> are the most compliant in Nb), the recrystallization mechanisms are examined based on the maximum energy release theory for recrystallization texture, i.e., the absolute maxium principal stress direction in the deformed grains becomes the minimum elastic modulus direction in recrystallized grains.

2:20 PM
Local and Polycrystalline Textures in BCC Metals: Their Evolution and Effect on Mechanical Response: *John F. Bingert*[1]; Benjamin L. Henrie[1]; Carl M. Cady[1]; George T. Gray, III[1]; Paul J. Maudlin[2]; [1]Los Alamos National Laboratory, MST-8, MS G755, Los Alamos, NM 87545 USA; [2]Los Alamos National Laboratory, T-3, MS B216, Los Alamos, NM 87545 USA

Texture development in BCC metals follows from the active deformation mechanisms and imposed strain path. Tensile, compressive, plane strain, and shear deformation induce different crystal rotations and thus resultant textures at both the macroscale and mesoscale. This work investigates the interaction of texture and bulk plasticity with regards to constitutive behavior, strain localization, and damage initiation in BCC metals. Tantalum and low-carbon steel were analyzed by electron backscatter diffraction to determine the crystallographic mesostructure, while mechanical testing was performed over a range of strain rates and temperatures. Polycrystal plasticity modeling was used to predict texture evolution for a suite of strain paths and to calculate multi-dimensional yield surfaces. The calculated yield surfaces were then applied to estimate texture effects on mechanical properties. Measuring the plastic anisotropy associated with experimental compression samples enabled validation of these simulations. The impact of relative slip system activity on anisotropic plasticity will also be explored.

2:40 PM

Texture Design in Achieving Desired Mechanical Properties in Cubic Materials: Jamaa Bouhattate[2]; *Dongsheng Li*[1]; Hamid Garmestani[1]; [1]Georgia Institute of Technology, Sch. of Matls. Sci. & Engrg., 771 Ferst Dr. NW, Atlanta, GA 30332-0245 USA; [2]Florida State University, Dept. of Mechl. Engrg., 2525 Pottsdamer St., Rm. 229, Tallahassee, FL 32310 USA

A processing path model for texture evolution based on a conservation principle in orientation space is applied to body-centered cubic materials. The model has been shown to represent texture evolution of materials during mechanical deformation. The streamlines derived from this model give a quantitative solution of the microstructure evolution during mechanical processing and provides the family of all possible processing paths from an arbitrary initial microstructure to the final microstructure with desired properties. This provides an inverse methodology which can empower the materials designer to take full advantage of the database in discovering the processing methods to achieve desired properties.

3:00 PM

Manipulating the Recrystallization Texture of Ferrite: *Matthew Robert Barnett*[1]; [1]Deakin University, Pigdons Rd., Geelong, VIC 3217 Australia

The typical recrystallization texture of commercial cold rolled steel is characterized by a strong fibre of grains with a {111} plane parallel to the rolling plane. The strength of this texture is sensitive to most of the adjustable material and processing variables. The presence of the {111} fibre texture is however, reasonably robust. One situation where departure from the typical recrystallization texture occurs is when the rolling temperature is around 700C, i.e. when warm rolling is performed. The present work examines this phenomenon through an analysis of a series of warm rolling experiments carried out on a number of low carbon and interstitial free (IF) steels. Electron Backscattering diffraction (EBSD) is employed to demonstrate that under certain conditions the {111} fibre grains in the deformed structure remain free of in-grain or micro-shear bands and that when this occurs {111} fibre textures fail to form during annealing. The role of Cr addition on this effect is also briefly examined. It is concluded that while in-grain type shear bands can generate unfavourable texture components under certain conditions, in warm rolled steels they appear to be essential for the generation of the commercially favourable {111} fibre recrystallization texture.

3:20 PM Break

3:40 PM

Effects of Oxygen on the Mechanical Behavior of Ta-10W: *E. P. George*[1]; J. R. DiStefano[1]; C. G. McKamey[1]; E. H. Lee[1]; [1]Oak Ridge National Laboratory, Metals & Ceram. Div., 1 Bethel Valley Rd., Oak Ridge, TN 37831-6093 USA

The effects of oxygen on the mechanical properties of Ta-10W are being investigated. Button-head tensile specimens were machined from recrystallized bar stock containing < 50 ppm oxygen. Oxygen concentrations up to ~1750 ppm were obtained by exposing the specimens at 1000°C to 5 x 10-6 torr flowing oxygen for various lengths of time, followed by a 1000°C heat treatment in vacuum for 8 h to diffuse and homogenize the oxygen. Total weight change after oxidation was measured to determine the amount of absorbed oxygen. Tensile tests were carried out in vacuum (~5 x 10-5 torr) at temperatures to 750°C. After fracture, the gage sections of selected specimens were chemically analyzed to determine the oxygen concentrations. The oxygen concentrations in the gage sections were found to be 1.36 ± 0.11 times the total weight change measured after oxidation due to the higher surface area to volume ratio in that region of the specimens. Relatively low concentrations of oxygen were observed to cause embrittlement at all the temperatures investigated; however, the critical concentration at which severe embrittlement occurred depended on the test temperature. Oxygen also caused significant strengthening. We will correlate the observed results with changes in hardness, fracture mode, and work hardening behavior. Research sponsored by the Office of Space and Defense Power Systems, U. S. Department of Energy, under Contract DE-AC05-00OR22725 with UT-Battelle, LLC.

4:00 PM

Transition Fracture Toughness of Low-Alloyed RPV Steels Before and After Irradiation: *Mikhail A. Sokolov*[1]; [1]Oak Ridge National Laboratory, Metals & Ceram., PO Box 2008, Oak Ridge, TN 37831-6151 USA

Prevention of reactor pressure vessel (RPV) failure in light-water-cooled nuclear power reactors depends primarily on maintaining the RPV material fracture toughness at levels that will resist fracture toughness, either brittle or ductile, during plant operation, including both normal and emergency conditions. A nuclear pressure vessel for use in pressurized water reactor (PWR) systems is designed to operate at pressures of about 15.5 MPa (2250 psi) and temperatures of about 288°C (550°F). The walls of a PWR vessel are made of ferritic steel sections up to 25 cm (10 in.) thick. Exposure of materials in light-water reactors to neutron irradiation may result in serious embrittlement, that can be marked by some significant increase in transition (brittle-to-ductile) fracture toughness temperature. The basic fracture toughness requirements are contained in Title 10, Code of Federal Regulations, Part 50, which references Section XI of the American Society of Mechanical Engineers (ASME) Boiler and Pressure Vessel Code. Section XI contains fracture toughness (K_{Ic}) curve as a function of temperature normalized to a reference nil-ductility temperature (RT_{NDT}). This curve was constructed as the lower boundary to the available in 1978 K_{Ic} database. Being a lower bound to the unique but limited database, the ASME K_{Ic} curve concept does not discuss probability matters. However, there has been a continuing evolution of fracture mechanics that has led to advances employing the Weibull distribution function to model the scatter of fracture toughness values in the transition range. The probabilistic-based estimates of median fracture toughness of ferritic steels tend to form transition curves of the same shape; namely, the so-called "master curve." The concept of universal master curve presumes a reference temperature based on the level of fracture toughness for the material. In the present study, the master curve concept is applied to large number of RPV steels before and after neutron irradiation. Radiation-induced increase in transition fracture toughness temperature is compared to the currently available regulatory procedures.

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The Effects of Proton Irradiation on the Compressive Properties of Tungsten at Room Temperature and at 475C: *Stuart Maloy*[1]; Chaitanya S. Deo[1]; Michael R. James[2]; G. J. Wilcutt[3]; M. Lopez[4]; T. J. Romero[5]; M. B. Toloczko[5]; [1]Los Alamos National Laboratory, MST-8, PO Box 1663, MS G755, Los Alamos, NM 87545 USA; [2]Los Alamos National Laboratory, AAA-TDO, MS H809, Los Alamos, NM 87545 USA; [3]Los Alamos National Laboratory, D-10, MS K575, Los Alamos, NM 87545 USA; [4]Los Alamos National Laboratory, NMT-11, MS G742, Los Alamos, NM 87545 USA; [5]Pacific Northwest National Laboratory, MS P8-15, PO Box 999, Richmond, WA 99352 USA

For the Advanced Fuel Cycle Initiative tungsten is being proposed as a backup solid target material to produce neutrons for the transmutation of long lived fission products. Previous work has shown that the mechanical properties of tungsten are degraded from irradiation in a fission neutron flux but little work has been performed on the irradiation of tungsten in a high energy proton beam. In this study, tungsten rods were irradiated at the 800 MeV Los Alamos Neutron Science Center proton accelerator for six months. After irradiation to a maximum dose in the tungsten of 23.3 dpa at Tirr=50-2700C, the tungsten was then sliced into short compression specimens (~3mm long). Hardness tests and compression tests were performed on the tungsten rods to assess the effect of irradiation on their mechanical properties. Results show an increase in the hardness and yield stress with increasing dose and decreasing test temperature. The observed results can be explained by the plastic anisotropy exhibited by bcc materials (including tungsten) caused by the geometry of the screw dislocation core. High Peierls barriers for the screw dislocation motion are a consequence of the asymmetric screw dislocation core; the motion of the screw dislocation in bcc metals is generally postulated to occur by the nucleation of double kinks (kink pairs) and subsequent migration and annihilation of the kinks. Irradiation causes an increase in the number of obstacles to dislocation motion and affects the energy barriers for double kink nucleation and kink migration on the screw dislocation. Kinetic Monte Carlo simulations of an idealized screw dislocation in a bcc metal are performed with attractive and repulsive solute configurations with energetics of the screw dislocation core taken from the literature. The observed yield stress and flow stress variation of the irradiated tungsten can be qualitatively explained by the variation of the single dislocation velocity with applied stress, impurity density and the strength of the impurity-dislocation interaction. Quantitative explanations require knowledge of the dislocation density and a detailed table of the nature of irradation induced debris and its interaction with the intrinsic dislocation network.

4:40 PM

Investigation of Portevin Le Chatelier Effect by Electrochemical Techniques: Correlations Between Dynamic Strain Aging and Metal-Elec-

trolyte Interface Potentials: *Ahmet Yilmaz*[1]; Dhanesh Chandra[2]; Raul B. Rebak[1]; [1]Lawrence Livermore National Laboratory, Energy & Environ. Direct., PO Box 5514, L-631, Livermore, CA 94551 USA; [2]University of Nevada, Metallurgl. & Matls. Sci. & Engrg., Mackay Sch. of Mines, Reno, NV 89557 USA

Portevin Le Chatelier (PLC) Effect is a phenomenon that occurs in many metals and alloys strained under certain rates and temperatures. It manifests itself by serrations of repetitive nature during plastic deformation. It is widely accepted that it occurs when mobility of diffused solutes such as C, N, and H was comparable to that of dislocations that creates repeated dislocation pile-ups and sudden stress releases. In this work, the potential of an electrochemical technique was examined for investigating the PLC effect that occurs in AISI 1020 low carbon steel strained at a rate of 10-6/s in dilute de-aerated aqueous electrolytes. Interface potential between the steel and the electrolyte was monitored as in-situ during creation, magnification, and annihilation phases of the serrated flow that was achieved by changing the specimen temperature in steps. The tests showed that initiation temperature of PLC effect in metals could be determined precisely by the technique. PLC effect in the low carbon steel was ini tiated at 55oC, with observable serrated flow of minimum amplitude. Experiments revealed precise correlations between the measured metal-electrolyte interface potentials and the serration amplitudes during the straining of the steel at the constant rate. The observed abrupt interface potential changes in the amount of 110 mV during creation of serrations showed that the dominant source of these changes was the dislocation-solute processes. The work showed the potential of the applied electrochemical technique as an experimental tool, to monitor and correlate PLC activities with interface potential, and also corresponding current under potentiostatically controlled interface potentials.

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Carbide Embrittlement in 4330 Modified Steel: *Donald Harold Sherman*[1]; Lawrence F. Allard[2]; [1]Caterpillar, Inc., Tech. Serv. Div., TCK/Div. 854, PO Box 1875, Mossville, IL 61656-1875 USA; [2]Oak Ridge National Laboratory, Matls. Analy. User Ctr., 1 Bethel Valley Rd., PO Box 2008, Oak Ridge, TN 37831-6064 USA

Depending on the processing path of Low Temperature Tempered medium carbon, low alloy steel components, a range of fracture toughness can occur. Fracture toughness specimens from commercial heats of 4330 modified steels were analyzed to determine fracture initiation processes and fracture modes as a function of both cooling rate and temper temperature. High resolution SEM and TEM analysis was done at Oak Ridge National Laboratory to determine size, location, distribution, morphology and identity of precipitates and phases present. The results show that microstructural changes in the martensite lath boundaries contribute directly to the fracture toughness.

Pb-Free and Pb-Bearing Solders: Session VI

Sponsored by: TMS - Electronic, Magnetic & Photonic Materials Division, TMS - EMPMD-Electronic Packaging and Interconnection Materials Committee

Program Organizers: C. Robert Kao, National Central University, Department of Chemical and Materials Engineering, Chungli City 32054 Taiwan; W. Plumbridge, Open University, School of Engineering Materials, Milton Keynes MK7 6AA UK; K. N. Subramanian, Michigan State University, Chemical Engineering & Material Science, East Lansing, MI 48824 USA

Wednesday PM — Room: Grand Ballroom K
September 29, 2004 — Location: Marriott New Orleans Hotel

Session Chairs: Yoshiharu Kariya, National Institute for Materials Science, Eco-Matls. Ctr., Tokyo 1088548 Japan; Mark A. Palmer, Ketterring University, IMEB, Flint, MI 48504 USA

2:00 PM Invited

Mechanical Properties of Lead Free Solder Alloys Evaluated by Miniature Size Specimen: *Yoshiharu Kariya*[1]; Tsuyoshi Asai[2]; Tadatomo Suga[3]; [1]National Institute for Materials Science, Eco-Matls. Ctr., Namiki 1-1, Tsukuba, Ibaraki 305-0044 Japan; [2]Shibaura Institute of Technology, Shibaura 3-9-14, Minato-Ku, Tokyo 1088548 Japan; [3]University of Tokyo, Rsch. Ctr. for Advd. Sci. & Tech., Nanometer-Scale Mfg. Sci. Lab., Komaba 4-6-1, Meguro-ku, Tokyo 153-8904 Japan

As solidified small volume Sn-3.0mass%Ag-0.5mass%Cu tensile specimen were fabricated to compare the mechanical behavior of the large volume versus the small volume specimen. It was found that tensile strength data for the small volume was not similar to that of the large volume, and clearly inferior to the large volume. The stress exponent of the small specimen was approximately 6.5 at 298K and 348K, which is smaller than that for large volume specimen. A value of 55kJ/mol was obtained for the activation energy from tensile tests of small volume specimen. This relates to the value of pipe diffusion controlled dislocation climb in pure tin. Detail of a fabrication procedure and mechanical properties of the small volume specimen will be presented.

2:30 PM

Role of Processing Variables on Mechanical Properties of Lead Free Solders: *Pranesh Aswath*[1]; Jonathan Rowley[2]; [1]University of Texas, Matls. Sci. & Engrg. Prog., 500 W. First St., Rm. 325, Arlington, TX 76019 USA; [2]U.S. Nuclear Regulatory Commission, Washington, DC 20555 USA

New experimental findings and analysis on the tensile fracture strength of solder joints made with the lead-free solder alloys 96.5Sn3.5Ag, 95.5Sn4.0Ag0.5Cu and 96.5Sn3.0Ag0.5Cu using convection reflow soldering techniques are reported. The employed specimens were all sandwiched solder joint assemblies subjected to multiple reflow soldering process variables: reflow temperature, reflow time, cooling rate and joint thickness. It was found that reflow time was the most important process variable in determining joint strength. The joint strength decreases rapidly with increasing reflow time. Cooling rates alter the reflow time, thus altering the joint strength. Faster cooling rates increased joint strength. Typically, a 20°C band in which peak reflow is to occur is used when processing electronic assemblies. Strength variations were found to be broad over such a band. Peak temperature needs to be precise to optimize strength.

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Special Boundaries and Deformation Mechanisms in Lead-Free Solder: *Adwait U. Telang*[1]; Thomas R. Bieler[1]; [1]Michigan State University, Chem. Engrg. & Matls. Sci., 2527 Engrg. Bldg., E. Lansing, MI 48823 USA

Orientation Imaging Microscopy (OIM) studies have shown that Sn-Ag based lead-free solder joints are multicrystals with several special boundaries, whose character is affected by the amount of alloying addition. These special boundaries could be affecting/assisting in the grain boundary sliding/ledge formation/decohesion that precedes crack formation. To investigate the correlation between special boundaries and deformation, a dual shear specimen was tested in TMF with external loads arising from differential thermal expansion between a Cu substrate and a nickel surface mount component; cycled at -15°C for 3.5 hr, followed by 20 minutes at 150°C. OIM revealed that multi-crystal solder joints with 7, 12.5, and 20° misorientation boundaries about <110> axes had corresponding ledges or grain boundary sliding evident in the SEM micrographs. The misorientation of these initial low angle grain boundaries increases with cycling, until they reach special low angle misorientations which can slide and/or crack, contrary to the conventional wisdom. This paper aims at inspecting such special boundaries in lead-free solder joints using SEM, OIM and TEM techniques to examine dislocation activity/solute atom segregation along these boundaries. Periodic grain boundary dislocations are needed to maintain low energy grain boundary structure and if these are glissile, sliding is likely. Such observations and analysis may explain how these deformation mechanisms account for damage evolution in lead-free solders.

3:20 PM

Tensile Strength of Composite and Non-Composite Lead Free Solders Using a Design of Experiments Approach: *Pranesh Aswath*[1]; Purushotham Kaushik[1]; Aravind Munukutla[1]; [1]University of Texas, Matls. Sci. & Engrg. Prog., 500 W. First St., Rm. 325, Arlington, TX 76019 USA

The tensile strength of composite and non-composite lead free solder joints are investigated in this study. Design of experiments was used in evaluating the role of various parameters like base alloy, reinforcement type, reinforcement percentages, reflow temperature, cooling conditions on the tensile strength of the solder joints. Two base alloys Tin/Silver binary eutectic (96.5Sn-3.5Ag) and Tin/Silver/Copper ternary (96.5Sn-3Ag-0.5Cu) are selected for this study. Cu and Ag (micron sized particles) are incorporated mechanically as reinforcement particles for composite solders. Scanning electron and optical microscopy were employed to analyze the fracture surfaces and microstructures of the solder joints after tensile testing. 96.5Sn-3Ag-0.5Cu has a higher strength as compared to 96.5Sn-3.5Ag with no reinforcements for different cooling conditions. When Cu or Ag is added to the base alloy as a reinforcement, the tensile strength of both binary and ternary alloys showed a reduction by about 30%. Aging studies are being conducted on both base alloys to know the effect of intermetallic growth on the mechanical strength of the solder joints.

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Mechanical Characterization of Bulk Sn-Bi Alloys and Sn-Bi-Alloy Solder Joints: *Mark A. Palmer*[1]; Samir Nashef[1]; Eric Coyle[1]; [1]Kettering University, IMEB, 1700 W. Third Ave., Flint, MI 48504 USA

In order to better understand thermal fatigue resistance, those more readily measured mechanical properties of materials are being determined.

Strength, creep and isothermal fatigue resistance of three different Sn-Bi alloys as a function of time and temperature have been measured. The properties of the bulk material will be compared to those of solder joints. These findings will be compared thermal fatigue resistance. Funding from the National Science Foundation CMS-0140605 is gratefully acknowledged.

4:25 PM Invited

Evaluation of Lead-Free Solders for Dissolution of Surface Metallization: *Ahmed Sharif*[1]; *Tan Chee Wei*[1]; Rashed Adnan Islam[1]; *Y. C. Chan*[1]; [1]City University of Hong Kong, Dept. of EE, 83 Tat Chee Ave., Kowloon Tong, Kowloon Hong Kong

Based on increasing pressures to achieve environmentally friendly electronic materials and processes, and indeed, growing governmental regulations around the world, the drive is strong to use lead-free solders in electronic assemblies. This push has highlighted the fact that the industry has not yet arrived at a decision for lead free solders. The reliability of the lead free solders has been studied a lot recently, but the knowledge of it still incomplete and many issues related to them are under heavy debate. This paper investigates three types of solder alloys, Sn/3Ag/0.5Cu, Sn/3.5Ag and Sn/0.7Cu used in a ball attached process. The scope of this paper covers lead-free solder system, comprehensively on Cu, electrolytic Ni/Au and electroless Ni/Au surface finish. This includes study on dissolution of under bump metallization (UBM), intermetallics at substrate-ball interface and activation energy computation. It was observed that Sn/0.7Cu solder had a melting temperature of around ten degrees above those of Sn/3.5Ag and Sn/3.8Ag/0.7Cu, which shows better dissolution behaviour than other lead-free alloys. A simplistic theoretical approach was also carried out to find out the amount of IMCs in the bulk of the solder by the measurement of the metal consumption from the substrate and the thickness of the IMCs that formed on the interface.

4:55 PM

Long-Term Aging Effects on Microstructure and Intermetallic Growth in Sn-Ag-Cu BGA Solder Joints: Adam Zbrzezny[1]; Leonid Snugovsky[1]; *Doug D. Perovic*[1]; [1]University of Toronto, Matls. Sci. & Engrg., Wallberg Bldg., 184 College St., Toronto, Ontario M5S 3E4 Canada

Lead-free (Sn-Ag-Cu) and Sn-Pb 256 PBGA components assembled with Sn-Ag-Cu and Sn-Pb eutectic solders on immersion Ag, electroless Ni/immersion Au, and Sn-Pb finished boards were subjected to isothermal aging at 125°C for 10000 hours. The solder joints were periodically analyzed with SEM/EDX for microstructural changes and with a BGA scope for surface roughness. The effects of aging on coarsening of the microstructure and on the morphology, growth kinetics and transformation of the intermetallic compound (IMC) layers were carefully evaluated. Special attention was paid to differences in metallurgies due to the joint formation on different board finishes. Finally, the implication of Pb presence in the Sn-Ag-Cu solder joints was thoroughly assessed and will also be presented.

5:20 PM

Solidifying Characteristics of Ni Particle-Reinforced Lead-Free Solder: *D. C. Lin*[1]; G.-X. Wang[1]; Y. Qiao[2]; T. S. Srivatsan[1]; [1]University of Akron, Mechl. Engrg., Akron, OH 44325-3903 USA; [2]University of Akron, Civil Engrg., 302 Buchtel Mall, Akron, OH 44311 USA

Eutectic Sn-3.5%Ag solder has been selected as a worldwide research topic for its most possible candidate to replace lead-bearing solders. Based on this popular solder, a series of experiments have been conducted to demonstrate that both micro-sized and nano-sized Ni powder additions can be effectively used as viable means for increasing the strength of eutectic Sn-3.5%Ag solder, even for a few percentages addition. This strength increasing is believed to be the result of intermetallic compound formation and background refining of eutectic structure. Microstructure observations have revealed that nanopowder Ni additions take different way in the matrix as comparing with microsized Ni powder. This presentation will highlight experimental observations on solidification characteristics of eutectic Sn-3.5%Ag solder, and composite solders which blended with both nanopowder and microsized Ni powder. The kinetics of both nucleation and growth of intermetallic compound during solidification will be discussed in order to understand the effect of Ni particle size on the microstructure development. Strength of the solidified product was quantified through tensile test. Results will reveal an increasing in strength and toughness of composite solders, with the addition of both nanosized and microsized Ni powder.

Titanium for Healthcare, Biomedical, and Dental Applications: Dental Applications and Phase Transformations-Microstructure

Sponsored by: TMS - Structural Materials Division, Japan Institute of Metals, TMS - SMD-Titanium Committee, TMS - SMD-Corrosion and Environmental Effects Committee-(Jt. ASM-MSCTS)

Program Organizers: Carl Boehlert, Alfred University, School of Ceramic Engineering and Materials Science, Alfred, NY 14802 USA; Dhanesh Chandra, University of Nevada, Metallurgical and Materials Engineering, Reno, NV 89557 USA; Masahiko Ikeda, Kansai University, Department of Materials Science and Engineering, Suita, Osaka 564-8680 Japan; Mitsuo Niinomi, Toyohashi University of Technology, Department of Production Systems Engineering, Toyohashi 441-8580 Japan

Wednesday PM Room: Mardi Gras Ballroom D
September 29, 2004 Location: Marriott New Orleans Hotel

Session Chair: Henry Rack, Clemson University, Sch. of Matls. Sci. & Engrg., Clemson, SC 29634 USA

2:00 PM Invited

Evaluation of Titanium Alloy with 1% Fe for Dental Applications: Marie Koike[2]; Chikahiro Ohkubo[3]; Hideki Sato[4]; Hideki Fujii[5]; Hiroyuki Fujii[2]; *Toru Okabe*[1]; [1]Baylor College of Dentistry, Texas A&M University Sys. Health Sci. Ctr., Biomatls. Sci., 3302 Gaston Ave., Dallas, TX 75246 USA; [2]Nagasaki University Graduate School of Biomedical Sciences, Removable Prosthodontics & Mgmt. of Oral Function, 1-7-1 Sakamoto, Nagasaki 852-8588 Japan; [3]Tsurumi University, Removable Prosthodontics, 2-1-3 Tsurumi, Tsurumi-ku, Yokohama 230-8501 Japan; [4]Tohoku University Graduate School of Dentistry, Operative Dentistry, 4-1 Seiryo-machi, Aoba-ku, Sendai 980-8575 Japan; [5]Nippon Steel Corp., Steel Rsch. Labs., 20-1 Shintomi, Futtsu, Chiba 293-8511 Japan

Good mechanical properties, biocompatibility, and corrosion resistance make titanium an excellent material for biomedical applications. However, when better mechanical properties than those of commercially pure (CP) titanium are needed, Ti-6Al-4V is sometimes used. Some new titanium alloys, developed as industrial structural materials, aim at an intermediate range of strength between that of CP Ti and Ti-6Al-4V. These alloys (Super-TIX800™, Nippon Steel Corp., Japan) contain iron (1%) with some adjustment of oxygen (0.30-0.35mass%) and nitrogen (0.005 to 0.04%). Besides being stronger than CP Ti, the cost of manufacturing these alloys is reportedly lower than of Ti-6Al-4V, and they do not contain aluminum or vanadium, which caused biocompatibility concerns in medical and dental appliances. It is worthwhile to evaluate how they compare to CP Ti and Ti-6Al-4V as candidates for dental use. We evaluated the tensile properties, corrosion characteristics, grindability, and mold filling capacity of these alloys with dental applications in mind.

2:25 PM Invited

Corrosiveness of Dental Treatment Agents on Dental Metallic Materials: *Yoshiki Oshida*[1]; Kawther Mirza[1]; Parul Agarwal[1]; Cory B. Sellers[1]; [1]Indiana University School of Dentistry, Dental Matls., 1121 W. Michigan St., Indianapolis, IN 46202-5186 USA

Currently, dental bleaching and fluoride treatments are popular for esthetic purposes as well as prevention and controlling plaque and carie formation. The corrosivenes of these treatment agents (normally containing hydrogen peroxide and fluoride) on dental metallic materials are not well documented. In this study, seven dental metallic materials including titanium materials were subjected to both treatment agents and the extent of corrosiveness were evaluated through chemical and electrochemical corrosion tests. It can be concluded that although these treatments are indicated for patients, it is proven that these agents are contraindicated for dental metallic materials.

2:50 PM Invited

Microstructural Modeling of Investment Cast Titanium for Dental Applications: *Robert C. Atwood*[1]; Peter D. Lee[1]; Richard V. Curtis[2]; Lucy Di Silvio[2]; [1]Imperial College London, Dept. of Matls., Prince Consort Rd., London SW7 2BP UK; [2]Guy's, King's College & St. Thomas's Hospital Dental Institute, Dental Biomatls. Sci., Floor 17, Guy's Tower, St. Thomas's St., London SE1 9RT UK

Titanium alloys are attractive materials for biomedical applications due to their superior biocompatibility. However, the use of titanium alloys for dental and maxillofacial prostheses is particularly challenging because each prosthesis has a unique, complex shape. A multiscale model for the processing of Ti prostheses was developed that combines a commercial macrocode for the process simulation with an in-house code to explicitly track the development of the microstructure including surface reactions. The model was applied to simulate the dental titanium investment casting process. The macroscopic filling and heat transfer is coupled with a microscale simulation incorporating the release and diffusion of impurity elements at the mould-metal interface. The penetration depth of oxygen and other species was simulated to determine the amount of alpha-case formed. The microstructural modeling results indicate that the critical factor is the time at which liquid Ti is in contact with the mould and that the incorporation of silicon from the mould increases this time.

3:15 PM Break

3:25 PM Invited
Phase Transformations in Ti-35Nb-7Zr-5Ta-(0.06-0.7)O Alloys: J. I. Qazi[1]; B. Marquardt[2]; *H. J. Rack*[1]; [1]Clemson University, Sch. of Matls. Sci. & Engrg., 213 Olin Hall, Clemson, SC 29634-0971 USA; [2]Zimmer Inc., Warsaw, IN 46581 USA

This investigation has examined the phase transformations occurring in Ti-35Nb-7Zr-5Ta-(0.06-0.7)O during aging between 260°C and 593°C. Solution treatment and cooling from above beta transus, approximately 800°C, resulted in retention of the beta phase, increasing O addition resulting in solid solution strengthening of the beta matrix. Increasing O content resulted in suppression of omega phase precipitation during aging at or below 427°C, only alpha precipitation being observed at the highest O level. Similarly when aging at or above 482°C, increasing O content resulted in enhanced alpha phase precipitation; no alpha phase precipitation being detected at the lowest O content examined after aging at 593°C for 8hrs. Finally with increasing O content the volume fraction of alpha phase increased with increasing aging temperature. This presentation will discuss these results by considering how O may suppress the beta to omega transformation while enhancing the beta to alpha + beta transformation.

3:50 PM Invited
Phase Transformations in Ti- (14-18 at%)Nb - (0.2-3.3at%)O Alloys: L. Monica Veca[1]; *H. J. Rack*[1]; [1]Clemson University, Sch. of Matls. Sci. & Engrg., Clemson, SC 29634-0971 USA

The phase transformations occurring in Ti-Nb-O alloys varying in chemical composition from 14 to 18 at% Nb and 0.2 to 3.3at% O following quenching from elevated temperature have been investigated. Characterization of the microstructure included X-ray diffraction, optical and transmission electron microscopy. It was observed that increasing Nb and O content both lead to a decrease in the martensite start temperature and an increase in the stability of the parent beta phase with respect to the omega transformation. While increasing Nb concentration had a larger effect on suppression of the beta to omega transformation, increasing O content resulted in a steeper decline in the martensite start temperature. This presentation will consider the effects of Nb and O content on the crystallographic description of the beta to martensite and the beta to omega transformations.

4:15 PM
Composition and Processing Dependence of Young's Modulus of Ti-Base Alloys for Biomedical Applications: *Guo He*[1]; Masuo Hagiwara[1]; [1]National Institute for Materials Science, Light Matl. Grp., 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047 Japan

Young's modulus is a very important property of artificial materials for implants. The mismatch in the elastic modulus of the implant and the natural bone is unfavorable for the bone healing and remodeling. A high elastic modulus of the implants results in bone resorption, while a low elastic modulus causes overloading. The Young's modulus of the implant should be as close as possible to that of the bone so that the implant will have isoelastic behavior corresponding to that of the bone. Ti-base alloys as biomaterials have excellent biocompatibility, low density, excellent corrosion resistance and good mechanical performance. However, the Young's modulus of Ti alloys with normal microstructure (beta, or alpha, or beta+alpha) is too high to compare with the natural bone. One of the concerns in recent studies on the bio-Ti alloys is to minimize elastic moduli while improving or maintaining other mechanical properties. In this presentation, we report the results on the composition and processing-dependence of Young's modulus of Ti-base alloys which show some possible methods to decrease the modulus.

4:40 PM
Relationship Between Tensile Deformation Behavior and Microstructure of Ti-Nb-Ta-Zr System Alloys: *Nobuhito Sakaguchi*[1]; Mitsuo Niinomi[1]; Toshikazu Akahori[1]; [1]Toyohashi University of Technology, Production Sys. Engrg., 1-1 Hibarigaoka, Tempaku-cho, Toyohashi, Aichi 441-8580 Japan

Ti-Nb-Ta-Zr system alloys composed of non-toxic elements have been expected to be used as biomaterials. In particular, newly developed Ti-29Nb-13Ta-4.6Zr conducted with a thermomechanical treatment has a possibility to show super elastic property and shape memory effect. Therefore, Ti-29Nb-13Ta-4.6Zr will be substituted for Ti-Ni system alloys. In the present study, relationship between tensile deformation behavior and microstructure of annealed Ti-XNb-10Ta-5Zr (X = 20, 25, 30 and 35) was investigated. Furthermore, the effect of cooling rate on tensile deformation behaviors of Ti-25Nb-10Ta-5Zr was also investigated.

5:05 PM
A New Titanium Alloy for Medical Application: *V. N. Zamkov*[1]; V. F. Topol'sky[1]; O. M. Ivasishin[2]; P. E. Markovsky[2]; [1]NAS of Ukraine, E.O. Paton Inst. for Elect. Welding Ukraine; [2]NAS of Ukraine, G. V. Kurdyumov Inst. for Metal Physics, 36, Vernadsky St., Kyiv 03142 Ukraine

New alloy of Ti-Al-Fe-Zr-Nb system has been designed for medical application. The primary goal was to substitute vanadium in a well-known Ti-6Al-4V composition, which is suspected to cause toxic damage to human body. On the other hand, the proposed alloy contains lower amount of expensive niobium as compared to a widely used Ti-6Al-7Nb composition. The alloy developed was melted with Electron-Beam Cold Hearth technique. Depending on thermomechanical processing and heat treatment employed, a wide range of mechanical properties was achieved. Tissue tolerance study was performed which showed a good biocompatibility, non-toxicity and high corrosion resistance of the alloy. Due to attractive balance of properties the alloy can be employed as material for dental implants, endoscopic tools, orthopedic implants, etc. Another version of this alloy with lesser amount of iron was also studied for applications where high strength can be sacrificed in the favor of ductility and corrosion resistance.

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