TIMIS Become A TMS Member

TMS derives its strength from its members, who take a hands-on approach to shaping the policy, programming, and publications of the society. Guided by these volunteers, TMS serves all segments of its professional community by:

FACILITATING NETWORKING:

By sponsoring numerous annual meetings and specialty conferences, TMS maximizes the opportunities for professionals from industries, universities, and government agencies worldwide to meet face to face and exchange technical ideas and experience, offer customer/client insights, find a mentor and/or serve as one, and just plain chat with peers and colleagues.

PRODUCING JOM AND OTHER PUBLICATIONS:

Every TMS member receives a complimentary subscription to JOM. Formerly Journal of Metals, this highly respected monthly journal, explores traditional, innovative, and revolutionary issues in the minerals, metals, and materials fields. Designed to be of maximum and immediate benefit to readers throughout the world, JOM is on-line before the print version is mailed.

TMS also publishes three other journals (*Journal of Electronic Materials* and *Metallurgical and Materials Transactions A and B*), numerous conference proceedings volumes and textbooks, and videos designed to give materials scientists and engineers the latest information on scientific and applied advances in areas as diverse as electronic materials, automotive manufacture, and extractive metallurgy.

PROMOTING LIFE-LONG LEARNING:

TMS is dedicated to the education of the materials science and engineering professional as well as to cultivating an interest in the field by young people.

For the practicing professional, TMS and its five technical divisions sponsor continuing education courses, primarily technical but also nontechnical, to promote the education and development of current and future professionals.

For student members, TMS participates on both the Accreditation Board for Engineering & Technology (ABET) and the National Council of Examiners for Engineering and Surveying (NCEES) to help, respectively, maintain the highest possible standards in the accreditation of metals and materials programs in academia and in the registration of professional engineers.

—All individuals registering for the 131st Annual Meeting & Exhibition at the non-member fee will automatically receive a one-year complimentary introductory membership for 2002. Your membership will be activated upon completion of your registration form, membership application, and payment of the non-member registration fee. You will receive a membership card and new member packet immediately after the meeting.

- Members from 77 countries and six of the world's seven continents.
- All new members will begin receiving a monthly subscription to JOM.

• New members will also be able to continue networking with a prestigious membership at future TMS meetings that fit their area of interest at a discounted member fee.

• Additional benefits include access to, and inclusion in the TMS Membership Directory on TMS OnLine at <u>www.tms.org</u>., professional development and continuing education opportunities, and group insurance programs. See the membership page on TMS OnLine for a complete list of membership benefits.

• Please direct any questions regarding your complimentary membership to the TMS Member Services Department via email to <u>castello@tms.org or via</u> phone to Margie Castello (724) 776-9000 Ext. 241.

TMS THE MINERALS, METALS & MATERIALS SOCIETY

PROMOTING THE GLOBAL SCIENCE AND ENGINEERING PROFESSIONS CONCERNED WITH MINERALS, METALS, AND MATERIALS

184 THORN HILL ROAD WARRENDALE, PA 15086-7514 USA

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THE VISION OF TMS IS TO BE THE PROFESSIONAL SOCIETY OF CHOICE FOR THE WORLDWIDE MINERALS, METALS AND

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- Five distinct technical divisions which are composed of 52 separate, highly specialized committees
- Periodicals: JOM, Metallurgical and Materials Transactions A and B, Journal of Electronic Materials
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FULL MEMBER

A candidate for election as full member shall be a person of integrity in activities associated with minerals extraction, processing, fabrication, or with materials applications. A candidate shall hold: (a) A baccalaureate degree in metallurgy, metallurgical engineering, materials science, or materials engineering, and at least 3 years' professional experience. (b) A baccalaureate degree in science or engineering in a discipline other than identified and at least 5 years' professional experience. (c) A baccalaureate degree from a recognized university in a discipline other than (a) or (b) and whose main activities lie in, but are not limited to, the development, management, administration, welfare, sales, or services to the minerals, metals and materials industries, with at least 7 years' experience. A credit in experience of one year for a masters degree or two years for a doctoral degree shall be granted. Annual dues: \$90.00

ASSOCIATE MEMBER

A candidate for associate member shall be a person of integrity who, while not possessing the academic or technical experience of a member, is active in fields that are sufficiently related to the advancement of, or service to, the minerals, metals or materials extraction, processing, or applications industry. Annual dues: \$90.00

The Minerals, Metals & Materials Society is a member society of the American Institute of Mining, Metallurgical and Petroleum Engineers, Inc.

ADMISSION REQUIREMENTS

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A candidate for election as life member shall be a person who qualifies as a full member or associate member and desires to only pay dues once.

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Pay dues once, effective for lifetime regardless of dues increase(s).

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The TMS membership year runs from January 1–December 31. Applications received January 1–September 30 will be processed for the current calendar year.

Applications received after September 30 will be processed for the remainder of the current calendar year and the entire following year. Membership benefits commence upon processing; subscriptions commence January–December of the following year.

Two weeks required for processing of complete applications submitted with full payment. Incomplete applications will not be processed. Allow eight to ten weeks for subscriptions to start.

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CONFERENCE PROCEEDINGS

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CALPHAD and Alloy Ther modynamics

Patrice E.A. Turchi, Antonios Gonis, and Robert D. Shull, editors These proceedings emphasize all theoretical aspects of computational thermodynamics and kinetics and their impact on the science of alloys and materials design. The book will provide an assessment of the CALPHAD (Calculation of Phase Diagrams) approach pioneered by 2002 Hume-Rothery Award recipient Larry Kaufman, a review of the current status of the software applications based on the CALPHAD approach, the impact of CALPHAD on alloy thermodynamics and design, and future prospects. The book will provide a detailed picture of the development of CALPHAD and point to further research. ISBN 0-87339-514-X

Approx. 390 pp., illus., index, hardcover

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Member price: \$72

Computational Modeling of Materials, Minerals, and Metals Processing

M. Cross, J.W. Evans, and C. Bailey, editors

This set contains the proceedings, in both print and CD-ROM formats, of the Computational Modeling of Materials, Minerals, and Metals Processing Symposium to be held at the 2002 TMS Annual Meeting in Seattle, Washington.

Computational models offer an effective way to design, analyze, and optimize materials, metals, and minerals processing. Computational modeling is increasingly becoming the means by which every factor in the operation of a process can be analyzed in a rational manner. Such models also represent a framework for much of our understanding of process operations.

This international symposium brings together participants from all aspects of computational modeling of materials, minerals, and metals processing, including the engineers involved primarily in specific applications, developers of computational modeling tools, and the developers of models. This allows all involved to understand the most recent advances in this rapidly developing enabling technology. ISBN 0-87339-513-1

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Creep Deformation: Fundamentals and Applications

Rajiv S. Mishra, James C. Earthman, and Sai V. Raj, editors

These proceedings focus on the application of fundamental creep research to the design and development of high temperature materials for engineering applications. The book deals with all aspects of creep deformation and high temperature materials development, specifically the influence of microstructures on various aspects of creep and the application of this information in the design of highly creep resistant materials. Emphasis will be placed on advanced crearanic and metal matrix composites and advanced intermetallics.

This volume brings together researchers working on fundamental issues relating to the development and characterization of high temperature materials and design engineers involved in high temperature applications. ISBN 0-87339-515-8

Approx. 415 pp., illus., index, hardcover Order No. 5158

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Light Metals 2002

Wolfgang Schneider, editor

Held at the TMS Annual Meeting & Exhibition each year, the Light Metals series has become the definitive annual reference source in the field of aluminum production and related light metals technologies. Each volume contains complete coverage of advancements and current work in cast shop technology, alumina and bauxite, carbon technology, aluminum reduction technology, and recycling. In addition, Light Metals 2002 includes coverage of reactive metals and advances in molten salt processing technology. Light Metals 2002 is sold as a package that includes the proceedings in both hardcover and text-searchable CD-ROM formats.

ISBN 0-87339-519-0

Approx. 1200 pp., illus., index, hardcover & CD-ROM

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EPD Congr ess 2002

Patrick R. Taylor, editor

The Extraction & Processing Division Congress, held at the TMS Annual Meeting & Exhibition each year, has become the definitive annual forum for new technological developments in the process metallurgy community. This volume will also include the proceedings of the Fundamentals of Advanced Materials for Energy Conversion symposium.

In addition to general abstracts, this year's edition will include papers on:

- Modeling of high temperature alloy processing
- General pyrometallurgy
- · Generation, treatment, metal recovery, and disposal of flyash
- Imaging of dynamic processes
- Materials processing fundamentals
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High-Cycle Fatigue, the David L. Davidson Symposium

Kwai S. Chan and Peter K. Liaw, editors

These proceedings from the David L. Davidson Symposium on High-Cycle Fatigue review the current research activities and assess the state-of-the-art in high-cycle fatigue, which has become a major concern in the design of engineering components and structures. This volume will include papers on a basic understanding of failure mechanisms, experimental methods and studies, modeling and simulation, and life-prediction methodology. This volume will also contain papers from the Fatigue of High Temperature Alloys Symposium, which deals with fatigue behavior of high temperature alloys, including crack initiation and propagation modes.

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High Per formance Metallic Materials for Cost-Sensitive Applications

F.H. (Sam) Froes and Lu Li, editors

These proceedings will examine the most recent advances and best practices in structural materials selection, design, and manufacturing for producing affordable components, with a focus on titanium, aluminum, and other advanced metallic materials. This volume will discuss melting, casting, powder metallurgy, forging, forming, extrusion, and machining, as well as processing advances, innovative processing techniques, process modeling and materials by design, new alloys, and related processing-microstructure-properties-performance-cost studies. ISBN 0-87339-522-0

Approx. 295 pp., index, PDF publication Order No. 5220 Member price: \$117

Sulfide Smelting 2002

Robert L. Stephens, and H.Y. Sohn, editors

These proceedings focus on all aspects of the pyrometallurgical production of primary metals from sulfide concentrates. Papers discuss industrial operations producing copper and nickel and the direct production of lead and zinc. Key topic areas include smelting and converting processes, recently completed capital projects, current operating practices, the predicted future of sulfide smelting operations, furnace integrity and refractory design, gas handling processes and equipment, issues related to the treatment of high-strength sulfur dioxide-containing off-gases, the production of alternative sulfur products, the treatment of acid plant blowdown streams and sulfated smelter dusts, and the capture and treatment of fugitive emissions.

ISBN 0-87339-525-5 Approx. 600 pp., illus., index, hardcover **Order No. 5255** Member price: \$70

Aluminum Reduction Technology: Magnetics and Modelling

Sponsored by: Light Metals Division, Aluminum Committee Program Organizers: Martin Segatz, VAW Aluminum AG, D-53117, Bonn Germany; Halvor Kvande, Norsk Hydro ASA, Oslo N-0240 Norway; Wolfgang Schneider, VAW Aluminium AG, Research & Development Manager Cast Technology, Bonn 53177 Germany

Thursday AM	Room: 6B
February 21, 2002	Location: Washington State Conv. & Trade Center

Session Chair: Marc Dupuis, GeniSim, Jonquiere, Quebec G7S2M9 Canada

8:30 AM

Magnetohydrodynamic (MHD) Analysis of Anode Change and Lowering of Anode: A Useful Tool for Analyzing the State of an Operating Pot: J. Antille¹; ¹Alcan Primary Metals Group Europe, CH 3965, Chippis Switzerland

A numerical simulation model solves the magnetohydrodynamic equations for the real geometries and bus bar arrangements of operating cells. This model predicts the natural oscillation frequencies of the cell observable in cell voltage and anode currents. The model calculates how an anode change and a lowered anode affect the natural frequencies. Measurements were made for a simulated anode change (simply isolating the anode), and for a real change (where material was deliberately allowed to sink and freeze to the cathode). The fluctuations of cell voltage and anode currents predicted were in good agreement with those measured in both cases, the frequency spectrum of the anode current indicating the presence or absence of bottom crust. Thus, analyzing the variations of anode current and/or cell voltage during normal operation can help in improving pot control.

8:55 AM

Metal Pad Roll Instabilities: *N. Ligonesche*¹; T. Lelievre²; J. F. Gerbeau³; C. Le Bris²; C. Vanvoren¹; ¹Aluminium Pechiney Research Center LRF, BP 114, 73300 Saint Jean de Maurienne France; ²CERMICS, Ecole Nationale des Ponts et Chaussees, 6 & 8 ave. Blaise Pascal Cite Descartes, Champs-sur-Marne, 77455, Marne La Vallee, Cedex France; ³INRIA, Projet M3N-Rocquencourt, BP 105, F-78153 Le Chesnay, Cedex France

The magnetohydrodynamic (MHD) phenomena which govern the movements of fluids (cryolite and aluminium) in Hall Heroult cells are extremely complicated. Indeed, the hydrodynamic and magnetic equations are closely coupled, through the Lorentz force (F = J \wedge B) and the induced currents $[J = (E + u^{\land} B)]$. One of the phenomena which is observed in industrial cells and which has been much investigated over the past few years is metal pad rolling. The aim of most of the theoretical and applied MHD studies of cell has been to understand, forecast and avoid this phenomenon. The originality of our approach consists in the choice of a variational formulation which is only based on the basic physical equations (Navier Stokes, Maxwell and Ohm's law) without any simplification or linearisation and in the way the coupling between the velocity and the magnetic field is naturally taken into account. Through our simulations, we have observed the phenomenon of metal pad rolling in a circular cell. Moreover, we have noticed that sufficiently small vertical field does not lead to instability, which shows that the nonlinear approach may usefully complement the linear one and slightly correct its conclusion in some situations.

9:20 AM

Modeling Power Modulation: *Marc Dupuis*¹; ¹GeniSim, Inc., 3111 Alger St., Jonquiere QC G7S 2M9 Canada

With, the recent power shortage in the USA, aluminum smelters are getting strong incentive to reduce their power consumption during peak demand. This power modulation can be quite harmful to the cells if not done properly. Yet, some smelters in Brazil are now successfully managing power modulation on a routinely basis following a long and expensive learning curve. Nowadays however, efficient dynamic cell simulator can be used in order to accelerate this learning curve and reduce the risk involved in performing power modulation without enough background experience. In this paper, two dynamic models are applied to study power modulation: an ANSYS based 2D+ full cell slice thermo-electric model and a much faster "lump parameter+" model.

9:45 AM

The Complex Mechanisms Inducing Anode Effects in Aluminium Electrolysis: *Helmut Vogt*¹; J. Thonstad²; ¹ TFH Berlin-University of Applied Sciences, Berlin D-13353 Germany; ²Norwegian University of Science and Technology, Dept. of Matls. Techn. and Electro.,7491Trondheim, Norway

The very fast increase in cell voltage manifesting the incipience of anode effects in industrial alumina reduction technology is the result of interactions of various processes. As evidenced by mathematical models, the decrese in wettability with decreasing alumina content, although shifting the current distribution to the side walls, raises the actual current density on the active area and affects mass transfer of reactant and product. The resulting voltage is accelerated with decreasing wettability. The anode effect occurs as the limiting current density on the wetted area is approached. The interpretation incorporates most, but not all, of the interpretations proposed during the past century.

10:10 AM Break

10:20 AM

Methodology of the Technico-Economical Analysis of the Potroom Activity: O. O. Rodnov¹; P. V. Poliakov¹; A. I. Berezin¹; P. D. Stont¹; ¹Scientific Technological Center, Light Metals, Post Box 14144, 95 Krasnoyarsky Rabochy St., Krasnoyarsk, 660025 Russia

It is necessary for smelters to have expert systems of analysis, which will permit to conduct deep evaluation of the technology of aluminum electrolysis with the purpose to determine the reasons, which provoke technology disturbances, to investigate and optimize operations. We offer methodology to analyze parameters of the potroom activity. This methodology establishes dependence between changes of the control actions and electrolysis parameters on one hand and amount of the produced aluminum, energy and raw materials consumption and economical figures on the other. Methodology includes 3 consecutive stages: 1. Preliminary preparation of the initial information (data base of the automatic system of management of the technological processes ASM TP), using classical statistical analysis as well as neural network technologies. This stage permit to evaluate the main dependences and interactions of the process. 2. Optimization of the process according to the technological criteria. We use the new method to built special simplex phase diagrams with criteria, which limits the area of optimization. Multi parametrical optimization with the purpose to investigate different regimes and to find out optimal control actions and parameters has been used. 3. Optimization according to the economical criteria including standard economical analysis where the results of the previous stage are used as input data for stage 3. The parameters of a real potroom have been analyzed. It was shown that decreasing or increasing target voltage resulted in aluminum production increase. Acceptable variant can be determined by economical analysis taking into account prices for energy, fluorides and other materials.

10:45 AM

Effect of Current Distribution on Current Efficiency in 160KA Prebake Cells: *Zeng Shuiping*¹; Zhang Qiuping¹; Ding Weian²; ¹North China University of Technology, Automation Inst., Beijing 100041 China; ²Beijing General Institute of Nonferrous Metal, Beijing 100041 China

This paper investigates the relations between the CE and the current distribution in 160KA prebake cells. On the bases of the viewpoint of zone current efficiency, a mathematic model to describe their relationship was established. And by use of cross design method, we simplified the relation and got a algebraic equation, which is the foundation to analyze the effect of current distribution on CE. Because both the current distribution and the current efficiency are uneven, the change of current distribution causes the change of CE, but not the strict even distribution gives the best CE, which is perhaps caused by uneven magnetic distribution. The paper also gives some suggestions to improve the cell operation and raise the CE.

11:10 AM

Study on Temperature Field and Incrustation of 160 KA Prebake Cells in the Guizhou Aluminum Smelter: Feng Naixiang¹; Sun Yang¹; *Li Hongpeng*²; Leng Zhengxu²; Feng Shaozhong²; ¹Academy of Materials and Metallurgy, Northeast University, Shenyang 11006 China; ²Guizhou Aluminum Smelter, Guiyang 550014 China

According to the measured results of the cell side temperature, the temperature field in the 160kA prebake anode reduction cell and the

coefficient of heat transfer between the incrustation and electrolyte melt, liquid aluminum were calculated by using finite element method and thermal flow pipe. From the calculated results, it can be seen that the coefficient of heat transfer between the incrustation and electrolyte melt, liquid aluminum is major. It was perhaps caused by unreasonable bus design, which can make the melt flow fast. In the present paper, the effects of using different inner lining materials and different cell voltage on the thickness of the incrustation, molecular proportion of electrolyte melt and current efficiency were calculated.

11:35 AM

Finite Element Analysis of Magnetohydrodynamics Stability of an Aluminium Reduction Cell: *Wu Jiankang*¹; Huang Ming¹; Huang Jun²; Yao Shihuang²; ¹Huazhong University of Science & Technology, Mech. Dept., Wuhan China 430; ²Guiyang Aluminum-Research Institute, Guiyang 550004 China

This paper employed finite element method to solve eigenvalues of 2D shallow-water perturbed magneto-hydrodynamic (MHD) system for stability analysis of an aluminum reduction cell. Stability analysis of 230 KA reduction cell was carried out in this paper. A series of frequency response figures of a reduction cell, which give disturbance growth rate and corresponding frequencies, was presented. The numerical results indicate that the presence of magnetic field always induces instability of a few long-wave modes of interface oscillations of electrolyte bath and aluminum liquid. meanwhile, the short-wave modes are stable. It is found that the growth rates of unstable modes strongly depend on current density, vertical magnetic field, mass density differences of electrolyte and molten aluminum, and liquid thickness of bath and molten metal. The numerical calculations confirm that the stability of reduction cell can be improved by increasing anode-cathode distance (ACD) and thickness of aluminum liquid.

Aluminum Sheet and Plate Rolling & Finishing Technology and Applications: Aluminum Sheet and Plate Applications

Sponsored by: Light Metals Division, Aluminum Association, Program Organizers: Michael H. Skillingberg, The Aluminum Association, Inc., Washington, DC 20006 USA; John P. Brandimarte, Precision Coil, Inc., Clarksburg, WV 26302-2650 USA; Karl Eminger, Alcoa, Inc., Alcoa Mill Products, Lancaster, PA 17604 USA; Seymour G. Epstein, The Aluminum Association, Inc., Washington, DC 20006 USA; Jeff J. Kadilak, Alcan, Inc., Oswego, NY 13126 USA; Leland R. Lorentzen, Nichols Aluminum, Davenport, IA 52801 USA; Douglas N. McLeod, ARCO Aluminum, Inc., Louisville, KY 40242 USA; Ken Schreckengast, Coastal Aluminum Rolling Mills, Inc., Williamsport, PA 17701 USA

Thursday AM Room: 608

February 21, 2002 Location: Washington State Conv. & Trade Center

Session Chairs: Douglas N. McLeod, ARCO Aluminum, Inc., 9960 Corporate Campus Dr., Ste. 3000, Louisville, KY 40242 USA; Michael H. Skillingberg, The Aluminum Association, Inc., 900 19th St. N.W., Washington, DC 20006 USA

8:30 AM Invited

Aluminum Sheet for Automotive Body Applications-Challenges and Opportunities: Andrew M. Sherman¹; ¹Ford Motor Company, 20000 Rotunda Dr., MD3182, Rm. 2160, SRL, Dearborn, MI 48121 USA

Over the past 25 years, motivated by the need to reduce vehicle weight in order to increase fuel economy, the use of aluminum in production automobiles has increased by more than 150%. Current average usage is about 250 pounds per vehicle; most of this, ca. 200 pounds, is in the form of castings. Applications of sheet include heat exchangers, heat shields, trim and a limited, but growing number of body panels (hoods, deck lids, fenders). While casting applications will continue to increase, by far the largest potential for growth in the use of aluminum is for body structures and closure panels. It has been shown that both closure panels and body structures can be designed to meet all vehicle requirements and that aluminum components can be manufactured in high-volume at rates the same as steel. However, a number of limitations remain: both material cost and manufacturing cost are higher, as are lead-time and investment. In addition, the infrastructure to support widespread application of aluminum bodies needs to be developed. This talk will outline some of the technical developments necessary to address these issues and discuss the elements of a long-range strategy for the cost-effective application of sheet aluminum in vehicles.

9:00 AM

The Global Market for Foil: Kelly J. Driscoll¹; ¹CRU International, Aluminium Grp., 31 Mount Pleasant, London WC1X 0AD UK

Foil is one of the principal end-uses for aluminium sheet. It has shown impressive growth rates in most developed world economies in recent years-but can that continue? In this paper we investigate historical trends and future growth prospects for foil production and consumption, analyse the threats to the foil market from substitution and the impact of recycling and legislation, and analyse the threats and opportunities posed by product innovation and down-gauging. We identify the major opportunities for growth, innovation, and new technologies.

9:30 AM

Opportunities for the Use of Aluminum in the Residential and Commercial Construction Markets: *Richard Bus*¹; ¹ATAS International, Inc., 6612 Snowdrift Rd., Allentown, PA 18106 USA Abstract Unavailable

Abstract Unavalla

10:00 AM Break

10:15 AM

Aluminum Applications in the Automotive Industry: *Richard L. Klimisch*¹; Joseph C. Benedyk³; Michael H. Skillingberg²; ¹The Aluminum Association, Inc., Detroit Office, One Towne Sq., Ste. 230, Southfield, MI 48076 USA; ²The Aluminum Association, Inc., 900 19th St. N.W., Ste. 300, Washington, DC 20006 USA; ³98 Schiller St., Lake Zurich, IL 60047 USA

An overview of recent developments and trends in the use of aluminum in the worldwide automotive industry is presented. Applications for various vehicle systems are discussed including those for the powertrain, structure, body and chassis. Recent developments in the production and assemby of aluminum automotive components, including the areas of forming and joining, are reviewed. The implications of the rapid growth of aluminum in automobiles is discussed as related to environmental sustainability, safety and vehicle performance. Aluminum's role in improving automotive fuel efficiency is addressed in light of the current heightened awareness of energy consumption.

10:45 AM

Enabling Communications about Aluminum Mill Products via Industry Standards: Peter Pollak¹; Parvaneh Shafiee¹; ¹The Aluminum Association, Inc., Techl., 900 19th St., N.W., Ste. 300, Washington, DC 20006 USA

Aluminum industry standards cover quantifiable attributes of aluminum mill products. They provide the basis of a common language for commerce and are an indispensable tool for communicating about aluminum alloys, tempers and mill products. The Aluminum Association promulgates the basic alloy and temper designation systems, which go through the American National Standards Institute's procedures for recognition as American National Standards. Even though there are several designation systems for different aluminum products (wrought, cast, primary, hardeners, etc), this paper focuses on standards for wrought mill products, and describes how the basic information is registered and is subsequently used in other codes and standards. Finally it covers the worldwide harmonization of aluminum industry standards, and how this is facilitated through international accords between the Aluminum Association, and its foreign counterparts.

11:15 AM

Studies of Chemical and Physical Emissions from Welding Aluminum Alloys: Seymour G. Epstein¹; ¹The Aluminum Association, Inc., 900 19th St. N.W., Washington, DC 20006 USA

Fabrication and repair of aluminum components and structures commonly involves the use of electric arc welding. In order to ensure the safety of the welders and others in the local environment, it is important to understand the nature of the chemical and physical emissions that are inherent to this joining process. Since aluminum is seldom used as the pure metal but is far more often alloyed with other metals to improve strength and various physical properties, the interaction of the arc and the metal being welded generates ultraviolet radiation, various metallica oxides and fumes, and gases. The exact composition of these emissions depends on the aluminum alloy(s) being welded. In order to provide needed data on welding emissions, The Aluminum Association sponsored several studies to characterize the emissions from arc welding by the metal inert gas (MIG) and tungsten inert gas (TIG) processes for various combinations of base and filler alloys. In some of the studies emissions from other processes, such as grinding and plasma arc cutting, were also investigated. In all cases the tests

were conducted to provide a means of estimating the "worst case" exposures.

Cast Shop Technology: Casting

Sponsored by: Light Metals Division, Aluminum Committee Program Organizers: David H. DeYoung, Alcoa Technical Center, Alcoa Center, PA 15069 USA; John F. Grandfield, CSIRO Australia, Preston, Victoria 3072 Australia; Wolfgang Schneider, VAW Aluminium AG, Research & Development Manager Cast Technology, Bonn 53177 Germany

 Thursday AM
 Room: 6A

 February 21, 2002
 Location: Washington State Conv. & Trade Center

Session Chairs: Christian Pluchon, Pechiney Group, Center Alp, BP 27, Voreppe 38341 France; Gary B. Parker, Wise Alloys LLC, Alabama Reclamation Ops., 1009 Ford Rd., Muscle Shoals, AL 35661-1119 USA

8:30 AM Keynote

D.C. Casting of Aluminium Alloys-Past, Presence, Future: *Wolfgang A. Schneider*¹; ¹VAW aluminium AG, R&D, Georg v. Boeselager Str. 25, Bonn 53117 Germany

The principles of D.C. casting of aluminium alloys were invented in 1936. Due to the importance of this process to the industry for the fabrication of semi-finished products intensive development work has taken place over the last 30 years. Increasing demands on ingot quality necessitated the development of innovative casting technologies. This has led, for example, to the introduction of air-assisted hot top moulds for the casting of extrusion ingots and electro-magnetic moulds for the casting of rolling ingots. Further techniques and tools were also developed to optimize the use of modern mould techniques and to increase the safety and reliability of the D.C. casting process. A review will be given of the history of D.C. casting and the state of the art of the process concerning casting technologies and ingot quality. Finally, future development trends and challenges will be discussed.

9:00 AM

The Manufacturing, Design and Use of a New Reusable Molten Metal Distributor for Sheet Ingot Casting: Sylvain P. Tremblay¹; Martin Lapointe²; ¹Pyrotek High Temperature Industrial Products, Inc., 1623 Manie St., Chicoutimi, Quebec G7K 1G8 Canada; ²Aluminerie de Becancour, Inc., 5555, Pierre-Thibault St., Ville de Becancour, Quebec G9H 2T7 Canada

In the last decade, the molten aluminum distribution in the ingot head of DC sheet casting ingots has been achieved using mostly a combo bag made of fiberglass fabrics. Some of these fabrics are openweave materials while others are solid fiberglass fabrics sewn together. This bag can deform and this can affect not only the distribution but also the molten metal temperature profile around the mold and at the end, the final ingot quality. This paper will review the use of a new distributor for DC sheet ingot casting. The paper is divided in two parts. The first part will deal with the principle and design of the new resusable molten aluminum distributor (ReMAD) to replace the standard combo bag. Description of the ReMAD materials used, presentation of water modeling and mathematical modeling experiments will complete the first part. Part two will present the test results of the ReMAD used at Aluminerie de Becancour Inc. (ABI) to cast AA-1045, AA-3003 and AA-5052. The following variables and measures will be discussed: Cast start-up, actual metal flow observations, ingot surface finish, temperature profile around the mold, ingot cut slice analyses, Podfa analyses and finally, results from the rolling plant. Comments from an operation point of view on the use of the reusable molten aluminum distributor will complete this presentation.

9:25 AM

On the Mechanism of Surface Cracking in DC Cast 7XXX and 6XXX Extrusion Ingot Alloys: *Steinar Benum*¹; Hallvard Fjaer²; Oddvin Reiso¹; Dag Mortensen²; Hilde Gunn Overlie¹; ¹Hydro Aluminium a.s., R&D Matls. Tech., PO Box 219, Sunndalsora N-6601 Norway; ²Institute for Energy Technology, Kjeller N-2027 Norway

When applying the Hydro variant of the Show Denko gas slip technology for casting of 7xxx alloys surface cracks occurred and gave a significant scrap rate in the cast house. Especially caused one alloy with 0.3 wt.% Cu problems. In order to identify the problem the casting process for this alloys were simulated by a coupled stress, thermal and fluid flow model (ALSIM/ALSPEN). The simulations were designed as a factorial trial where casting speed, ramping of the speed, casting temperature, cone height of the starting block, cooling water efficiency and primary cooling were varied systematically. The hoop stress in the surface at the temperature when 95% of the material was solidified was used as a crack sensitivity indicator. Three stages were found: (I) At the start a maximum hoop stress evolved, (II) then a minimum stress occurred (III) before the stress reached a stable level. For an AA6xxx alloy the stress was found to be zero in the stable stage while the 7xxx alloy had tension stresses during the stable stage. Based on the factorial analysis it was found that the stable stress increased with increasing casting speed and decreased with an increased primary cooling. Furthermore, the initiation and propagation of cracks are discussed based on investigations on real cracks. Here it was found that cracks tended to initiate when oxide lumps were released from the hot top.

9:50 AM

Nature and Formation of Surface Cracks in DC Cast Ingots: *Qingyou Han*¹; Srinath Viswanathan¹; Douglas Spainhower²; Subodh K. Das³; ¹Oak Ridge National Laboratory, Metals & Cer. Div., PO Box 2008, Oak Ridge, TN 37831-6083 USA; ²Logan Aluminum, Inc., PO Box 3000, Russelville, KY 42276 USA; ³Secat, Inc., 1505 Bull Lea Blvd., Lexington, KY 40511 USA

Surface cracks are critical defects that increase the cost and reduce the yield of the DC casting process. However, there is some debate about the nature of surface cracks in the literature. In this study, surface cracks on a 3004 alloy ingot were examined in detail. Optical microscopy showed that the crack occurred along grain boundaries. Dendrites were clearly seen on the fracture surface using Scanning Electron Microscopy. Auger analysis indicated that silicon and magnesium were highly segregated on the fracture surface. When coupled with a simulation of the solidification of 3004 alloy, the results suggest that the surface cracks that occur during DC casting of aluminum alloys are hot tears that form above the solidus temperature, rather than cold cracks that form below the solidus temperature.

10:15 AM Break

10:30 AM

Experimental Study of the Heat Transfer along the Surface of a Water-Film Cooled Ingot: *Laszlo Istvan Kiss*¹; Thomas Meenken¹; Andre Charette¹; Yves Lefebvre²; Robert Levesque³; ¹Universite du Quebec a Chicoutimi, Dept. des Sciences Appliquees, 555 blvd. de l'Universite, Chicoutimi, Quebec G7H 2B1 Canada; ²Betz-Dearborn Canada, Inc., 3451 Erindale Station Rd., Mississauga, Ontario L5A 3T5 Canada; ³Alcoa Baie-Comeau, 1001 Rt. Maritime, Baie-Comeau, Quebec G4Z 2L6 Canada

In the recent years many research efforts have been directed toward the determination of the heat transfer coefficients between the solidifying ingot and cooling water during the semi-continuous casting of aluminum ingots. The present study aims to the analysis of the influence of water quality and ingot properties on the cooling capacity. An experimental technique was developed to follow closely the variations of the surface heat flux without modifying the surface properties of the solid. The results are presented in the form of surface heat flux vs. surface temperature and heat transfer coefficient vs. temperature diagrams. The correlation between the different definitions of local and average heat flux coefficients is discussed.

10:55 AM Cancelled

The Formation of Surface Segregates during Twin Roll Casting of Aluminium Alloys: Børge Forbord

11:20 AM

Thixoforming Raw Material Development by Means of Optimized Design of Experiments (DoE): *T. Noll*¹; B. Friedrich¹; ¹IME-Metallurgische Prozesstechnik und Metallrecycling, RWTH Aachen, Intzestraße 3, 52056 Aachen Germany

Thixocasting and Forging belongs to modern forming processes. The process is a soft forming process in which semi solid slurries with a stiffness of "butter" can be formed under low pressure and temperature substantially lower than those used for casting. Thixoforming gains an increasing interest. The automobile industry-for examplelooks for process technology which connect complex parts with improved mechanical properties. Potential of energy- and costs-saving is not to be neglected. Although this process was already developed in 1972 by MIT (Massachusetts Institute of Technology, Cambridge) the required improvement of process stability and the introduction of suitable quality management systems must be improved. Progress in process stability should start with raw material development. The first part of this paper is a stock taking and gives an introduction into the Thixoforming process and its typical process steps. The most important technologies of raw material preparation will be presented, too. In the second part of this paper raw material development by chemical grain refinement and determination of suitable DC-casting process parameters by means of optimized design of experiments will be presented.

11:45 AM

Automatic Bleedout Detection System Leading Safety Development: *Todd Snyder*¹; Andrew J. Widrig¹; *Helmut Suppan*²; ¹Wagstaff, Inc., 3910 N. Flora Rd., Spokane, WA 99216 USA; ²Aluminium Ranshofen Huttengiesserei Ges.m.b.H., Postfach 35, Lambrechtshausner Strasse, Braunau, Ranshofen A-5282 Austria

As total production dynamics in the casthouse changes, principally to higher capacity equipment with reduced exposed man hours per ton produced, Wagstaff, Inc., has successfully introduced the StopCast(TM) Automatic Bleedout Detection System and plug off mechanism to the industry. This paper will outline the operational details of the StopCast system and share experiences from our first installation at Aluminium Ranshofen Hüttengiesserei Ges.m.b.H.

Charles J. McMahon Interfacial Segregation and Embrittlement Symposium: Design of New Materials

Sponsored by: ASM International: Materials Science Critical Technology Sector, Structural Materials Division, Materials Processing & Manufacturing Division, Jt. Mechanical Behavior of Materials, Jt. Computational Materials Science & Engineering, Texture & Anisotropy Committee

Program Organizers: Vaclav Vitek, University of Pennsylvania, Department of Materials Science and Engineering, Philadelphia, PA 19104 USA; Clyde Briant, Brown University, Division of Engineering, Providence, RI 02912 USA; Harvey D. Solomon, General Electric Company, Research & Development Center, Schenectady, NY 12309 USA

 Thursday AM
 Room: 307-308

 February 21, 2002
 Location: Washington State Conv. & Trade Center

Session Chairs: John Knott, University of Sheffield England; David Embury, McMaster University, Matls. Sci. & Eng., 1280 Main St., W., Hamilton, Ontario L8S 4L7 Canada

8:30 AM Invited

The Electrochemical Fatigue Sensor-Development Update: Y. F. Li¹; J. Wang¹; M. Wang¹; A. Witney¹; J. DeLuccia¹; *Campbell Laird*¹; ¹University of Pennsylvania, Dept. of Matls. Sci. & Eng., 3231 Walnut St., Philadelphia, PA 19104 USA

The Electrochemical Fatigue Sensor (EFS) has undergone considerable development for commercial purposes in the last three years, and advances have been made in both understanding its mechanism and in applying it. The present understanding by which the sensor current responds to mechanical stress and fatigue damage is described and an up-to-date description of the developed device is presented. Since the EFS gives real time information about the state of damage in a specimen undergoing fatigue, it offers considerable advantage as a laboratory tool for understanding fatigue mechanisms. Examples of its use in studying small crack growth behavior and in cumulative damage under variable loading are provided.

9:05 AM Invited

Advanced Metal Science Based on Nano-Metallurgy: Kenji Abiko¹; ¹Tohoku University, Inst. for Matls. Rsrch., 2-1-1 Katahira, Aoba, Sendai, Miyagi 980-8577 Japan

We have carried out the fundamental research of ultra-high purity metals which were melted by a newly designed induction-melting furnace with a cold copper crucible using ultra-high vacuum technology. The purity of Iron melted is analyzed to be higher than 99.9989 mass%. The ultra-purified iron possesses the incredible properties such as mechanical properties, deformation behavior, corrosion resistance and so on. These experimental results can not be predicted from the conventional metallurgy. It is concluded that the "Nano-Metallurgy" which is the metallurgy based on the ultra-purification and the microstructure control of metals in nano-scale is effective to find the inherent properties.

9:40 AM Invited

Grain Boundary Engineering for Alleviating Weld Sensitization and Stress Corrosion Cracking in Nickel-Based Alloys: Gino Palumbo¹; ¹Integran Technologies, Inc., 1 Meridian Rd., Toronto, Ontario M9W 4Z6 Canada

Advances in the modeling of microstructural evolution and in material characterization techniques (e.g., automated electron diffraction) have led to the emergence of innovative and cost-effective thermomechanical processing methods for the control and optimization of grain boundary structures in conventional polycrystalline materials; these processing methods being designed to yield increased populations of structurally-ordered high angle grain boundaries in the microstructure. In this presentation, an overview of the theoretical basis and the practical application of grain boundary engineering concepts to the design and development of high performance Nickelbased alloys (e.g., 600, 625, 690, 738, 800, C-22 etc.) will be presented and discussed. The grain boundary engineering approach is shown to enhance the resistance of these alloys to weld sensitization, intergranular corrosion and stress corrosion cracking, and can be used to improve component reliability and extend service life in numerous applications (e.g., nuclear plant components, nuclear waste storage, recovery boilers, combustion turbines etc.)

10:15 AM Invited

Materials by Design: Quantum Steel: Gregory B. Olson¹; ¹Northwestern University, Dept. of Matls. Sci. & Eng., 2225 N. Campus Dr., Evanston, IL 60208 USA

A systems approach integrates process/structure/property/performance relations in the computational design of materials as multilevel dynamic structures. For the case of ultrahigh-strength martensitic steels, quantum mechanical total energy calculations using the FLAPW method address the thermodynamic and electronic basis of segregation effects on grain boundary cohesion identified by McMahon and coworkers. Model predictions of cohesion enhancing components are integrated with a set of microstructural design models to design a first generation of Quantum Steels exploiting quantum mechanical predictions to enhance resistance to intergranular hydrogen stress corrosion cracking. Research performed in collaboration with W-T. Geng, A.J. Freeman and C. Kantner under ONR sponsorship.

10:50 AM

Grain-Boundary Segregation of Trace Elements in Iridium Alloys and Effects on Mechanical Properties: *E. P. George*¹; L. Heatherly¹; C. T. Liu¹; ¹Oak Ridge National Laboratory, Metals & Cer. Div., 1 Bethel Valley Rd., PO Box 2008, Oak Ridge, TN 37831-6093 USA

Iridium is attractive for high-temperature structural applications because of its high melting point and good oxidation/corrosion resistance. A major drawback is its low tensile ductility when tested at conventional strain rates at low temperature, and at high strain rates at elevated temperature. Microalloying has been used to strengthen the grain boundaries and suppress brittle intergranular fracture in Ir alloys. Auger studies indicate that Th and Ce have a strong tendency to segregate to Ir grain boundaries and suppress intergranular fracture at elevated temperatures. We review here the properties of the Th-doped alloys that have been successfully developed for space power applications at temperatures to 1400°C as well as the Ce-doped alloys that are currently under development for future applications. We will also discuss the grain-boundary segregation of Si and its role in the severe embrittlement of iridium alloys. Research sponsored by the Office of Space and Defense Power Systems and the Division of Materials Science and Engineering, US Department of Energy under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

11:10 AM

Failure Mechanisms of Thermal Barrier Coatings-Effect of Alloying Elements and Impurities: *Jeff Pfaendtner*¹; Irene Spitsberg¹; ¹GE Aircraft Engines, Matls. & Proc. Eng. Dept., One Neumann Way, MD M89, Cincinnati, OH 45215 USA

The chemical and thermo-mechanical factors leading to spallation of EB-PVD Thermal Barrier Coatings (TBC) from platinum-aluminidecoated nickel-superalloy substrates are discussed. Reactive element and refractory element diffusion into the bond coat from the substrate during cyclic high-temperature exposure are shown to have a strong effect on TBC spallation life. This effect can result in a significant increase in TBC life depending on the superalloy used as substrate. The presence of interstitial impurities in the bond coat has been shown to counteract the effectiveness of these substrate elements. The effect of these diffused elements on the major components of the mechanism of TBC failure, e.g. growth rate and adhesion of the thermally growth oxide (TGO), and ratcheting of the TGO/bond coat interface, will be discussed.

11:30 AM

Evolution of Grain Boundary Planes in Grain Boundary Engineering: *Christopher Schuh*¹; Mukul Kumar¹; Wayne E. King¹; Lan Nguyen¹; ¹Lawrence Livermore National Laboratory, Matls. Sci. & Tech., 7000 East Ave., L-350, Livermore, CA 94550 USA

The process of grain boundary engineering, whereby the fraction of "special" grain boundaries is increased through sequential thermomechanical processing, gives rise to considerable improvements in, e.g., intergranular cracking resistance, intergranular corrosion resistance, creep strength, and ductility of low to medium stacking fault energy FCC metals. The special properties of such grain boundaries are usually correlated only with the relative misorientation across the boundary, and neglect the plane of the boundary with respect to the crystallographic axes of the two grains. In the present work, we describe experiments on a nominal Ni-Cr-Fe solid solution alloy in which both of these geometrical parameters are measured using electron backscatter diffraction orientation mapping on serial sections. Specifically, we explore the effect of thermomechanical processing on the evolution of both the misorientation and the plane of grain boundaries. The results are discussed in the context of the crystallographic constraint imposed by the triple junctions and their connectivity.

Computational Phase Transformations: Computational Materials Design

Sponsored by: ASM International: Materials Science Critical Technology Sector, Electronic, Magnetic & Photonic Materials Division, Structural Materials Division, Chemistry & Physics of Materials Committee, Jt. Computational Materials Science & Engineering, Thermodynamics & Phase Equilibria Committee *Program Organizers:* Long-Qing Chen, Pennsylvania State University, Materials Science and Engineering Department, University Park, PA 16802-5005 USA; Mark Asta, Northwestern University, Department of Materials Science and Engineering, Evanston, IL 60208-3108 USA; Zi-Kui Liu, Pennsylvania State University, Materials Science and Engineering, University Park, PA 16082-5005 USA; James Aaron Warren, NIST, CTCMS and Metallurgy Division, Gaithersburg, MD 20899-8554 USA

Thursday AM	Room: 201
February 21, 2002	Location: Washington State Conv. & Trade Center

Session Chair: Zikui K. Liu, Pennsylvania State University, Matls. Sci. & Eng., University Park, PA 16802 USA

8:30 AM

Transformation Modeling in Computational Materials Design: Greg B. Olson¹; H.-J. Jou²; ¹Northwestern University, Dept. Matl. Sci. & Eng., 2225 N. Campus Dr., Evanston, IL 60208 USA; ²QuesTek Innovations, LLC, 1820 Ridge Ave., Evanston, IL 60201 USA

A range of dynamic models based on the Thermocalc/DICTRA system is applied in the computational design of materials as dynamic multilevel structures. For the case of complex multicomponent martensitic steels, a kinetic model predicting Ms temperatures has been extended by G. Ghosh to predict the full evolution of lath martensite microstructures controlling retained austenite content. A model of bainitic transformation as a coupled diffusional/displacive mechanism predicts bainite-start C-curves for control of hardenability. The new PrecipiCalc software for simulation of precipitation reactions based on the Langer-Schwartz framework is being applied to the simulation of precipitation hardening of Ni-base aeroturbine disc alloys under an initiative aimed at acceleration of the full materials development and qualification cycle.

9:15 AM

Calphad and the Phase-Field Method: John Ågren¹; ¹KTH, Matls. Sci. & Eng., Stockholm SE-100 44 Sweden

The phase-field method has been tremendously successful in generating realistic micro structures, e.g. dendrites during solidification and different variants of martensite. It is possible to take various factors like stresses and crystallographic anisotropy into account. However, so far mostly very simple and not very realistic systems have been treated, e.g. heat flow in pure substances, isothermal diffusion in binary systems etc. Unfortunately, the materials properties have been rather far from those of real multi-component alloys. The phase-field community has thus not made much use of the recent advances in thermodynamic modelling and high-quality databases presented within the Calphad community. Nevertheless, the governing equations of the phase field-method may be derived from the Gibbs energy of entropy functions given by the Calphad method. The most severe difficulty when coupling thermodynamic softwares to phase-field computations is the computational speed. In this presentation the basic theory will be reviewed and some recent applications will be discussed. Different ways of increasing the computational speed will be discussed.

9:45 AM

Linking Phase-Field Model with CALPHAD: Application to Morphological Evolution of Gamma-Prime Precipitates in Ni-Base Alloys: *Jingzhi Zhu*¹; V. Vaithyanathan¹; Z. K. Liu¹; L. Q. Chen¹; ¹Pennsylvania State University, Matls. Sci. & Eng., University Park, PA 16802 USA

This presentation reports our preliminary results of a multi-year effort in developing a set of computational tools for modeling the thermodynamics, microstructure evolution, and mechanical properties of Ni-base superalloys. In particular, we describe a phase-field model which has the following unique features: (1) it uses a local free energy as a function of composition and order parameters directly constructed using the semi-empirical CALPHAD method; (2) it employs an efficient iterative method for solving the elastic equations for elastic inhomogeneous systems; (3) it takes into account the composition and order parameter dependence of atom mobilities; and (4) the kinetic equations are solved using an efficient semi-implicit Fourier-spectral method. With all the important thermodynamic and kinetic parameters either from a database or from independent experimental measurements, the three-dimensional morphology of gammaprime (Ni3Al) precipitates in a disordered fcc matrix is studied as a function of precipitate size. Results from the simulation are compared with existing experimental observations in Ni-base alloys. The work is supported by NASA.

10:05 AM Break

10:15 AM

Development of Multicomponent Diffusion Mobility Databases: C. E. Campbell¹; ¹NIST, Metall., 100 Bureau Dr., MS 8555, Gaithersburg, MD 20899-8555 USA

As the demand for improved materials performance and processing efficiency increases, a better understanding multicomponent multiphase diffusion has become essential. One of the first steps in this process is the assembling of diffusion mobility databases, which can be used with thermodynamic databases to calculate composition-dependent diffusivities. The mobility databases are constructed using a CALPHAD approach that assumes that quaternary and higher order interactions can be neglected allowing binary and ternary assessments to be combined to extrapolate to higher order systems. Construction of a Nibased diffusion mobility database is used to demonstrate the database development process, which includes the analysis of available diffusion data, the assessment of diffusion activation energies in metastable states, and the validation of the extrapolation to higher order systems. Finally, comparison of measured and simulated composition profiles from a diffusion couple of two commercial superalloys allows the nonmonotonic diffusion behavior predicted by the composition-dependent diffusivities to be evaluated.

10:45 AM

Some Attempts of Hybridized Calculation of Phase-Field Method and Cluster Variation Method: M. Ohno¹; *T. Mohri*¹; ¹Hokkaido University, Div. of Matls. Sci. & Eng., Grad. Sch. of Eng., Sappro 060-8628 Japan

In order to gain both atomistic and microstructural evolution processes, a hybridized calculation of Cluster Variation Method and Phase-Field Method is attempted. Particular focus is placed on disorder-B2 and disorder-L10 transitions. In addition to microstructural evolution process, atomistic evolution process is visualized based on the time evolutions of cluster correlation functions obtained by CVM. The distinctive feature of existence(L10) and non-existence(B2) of triple point at Anti Phase Boundary is confirmed. Furthermore, the relaxation behavior of Long Range Order parameter is critically examined and is compared with the one obtained by Path Probability Method.

11:05 AM

Microstructure Simulations of a 5-Component Ni-Base Model Alloy: *Nils Warnken*¹; Bernd Boettger¹; Dexin Ma¹; Victor Vitusevych¹; Nathalie Dupin²; Suzana Gomes Fries¹; ¹ACCESS e.V., RWTH-Aachen, Intzestr. 5, Aachen D-52072 Germany; ²Calcul Thermodynamique, 3, rue de l'avenir, Orcet F-63670 France

In order to investigate solidification microstructure and microsegregation in Ni base superalloys, a model alloy containing the five elements Ni, Cr, Al, Ta and W was designed and produced. Directional solidified samples were prepared in a Bridgman type furnace to provide the benchmark data for the simulations. The simulations are done using the ACCESS Multiphase, Multicomponent Phase Field Model, coupled to a thermodynamic database. The same model is also applied to simulate the homogenization of the cast structure during heat treatment. The simulation results show reasonable agreement with the solidification experimental data for the formation of the primary (A1) and secondary phases (L12). Equilibrium experiments are being performed in order to fine tune the thermodynamic database. This work has been done within the Collaborative Research Center 370 "Integrated Modeling of Materials" of the Deutsch Forschungsgemeinschaft (DFG).

11:25 AM

A Pseudo-Front Tracking Technique for the Modelling of Solidification Microstructures in Multi-Component Alloys: Alain Jacot¹; Michel Rappaz¹; ¹Ecole Polytechnique Fédérale de Lausanne, LMPH, EPFL, MX-G, Lausanne 1015 Switzerland

A two-dimensional model for the simulation of microstructure formation during solidification in multi-component systems has been developed. The model is based on an new pseudo-front tracking technique to describe the evolution of interfaces that are governed by solute diffusion and Gibbs-Thomson effect. The diffusion equations are solved in the primary solid phase and in the liquid using an explicit finite volume method formulated for a regular hexagonal grid. The interface curvature is obtained from the field of the signed distance to the interface and a PLIC (Piecewise Linear Interface Calculation) technique, which allows to reconstruct the position of the interface in these mushy volume elements. The concentrations at the solid-liquid interface are calculated using thermodynamic data provided by the phase diagram software Thermo-Calc. Different coupling strategies between the microstructure model and Thermo-Calc have been developed, in particular a computationally-efficient direct coupling using the TQ-interface of Thermo-Calc. After testing the accuracy of the model with respect to solute and curvature calculation, comparisons are made with predictions obtained with the marginal stability theory, a 1D front-tracking method and 2D phase-field simulations of dendritic growth in binary alloys. The model is then used to describe the formation of several grains in an Al-1%Mg-1%Si alloy, as a function of the heat extraction rate and inoculation conditions. It is shown that the model is capable of reproducing the transition between globular and dendritic morphologies.

11:45 AM

High-Speed Thermodynamic Calculations for Kinetic Simulations: *Henrik Strandlund*¹; ¹Royal Institute of Technolgy, Div. of Physl. Metall./Dept. Matl. Sci. & Eng., Brinellvagen 23, Stockholm 100 44 Sweden

Simulation of phase transformations may be divided into two parts; the simulation of kinetics and the calculation of thermodynamic quantities. A number of softwares for thermodynamic calculations are available and it is thus convenient to use such software to obtain an accurate description of thermodynamic properties and couple them to a software simulating the kinetics. A major problem then is that the computational work to evaluate the thermodynamic quantities is too heavy unless very simplified thermodynamic models are used. That problem may be solved by calculating the thermodynamic quantities in selected points and time steps only and apply an artificial neural network to obtain the values in all other points. This approach has successfully been applied to diffusion in alloys and examples will be given showing how this approach enables us to incorporate thermodynamic data from Thermo-Calc into simulations of diffusion in a very efficient way.

Deformation and Stresses in Small Volumes: Fatigue and Fracture of Small Volumes

Sponsored by: ASM International: Materials Science Critical Technology Sector, Structural Materials Division, Jt. Mechanical Behavior of Materials

Program Organizers: David F. Bahr, Washington State University, Department of Mechanical & Materials Engineering, Pullman, WA 99164-2920 USA; Eric Kvam, Purdue University, School of Materials Engineering, West Lafayette, IN 47907-1289 USA; Scott X. Mao, University of Pittsburgh, Department of Mechanical Engineering, Pittsburgh, PA 15261 USA; Neville R. Moody, Sandia National Laboratories, Livermore, CA 94551-0969 USA

Thursday AM	Room: 303
February 21, 2002	Location: Washington State Conv. & Trade Center

Session Chair: Gene A. Lucadamo, Sandia National Laboratories, PO Box 969, MS 9161, Livermore, CA 94551-0969 USA

8:30 AM Invited

On the Mechanism of High-Cycle Fatigue in Si Thin Films for MEMS Devices: C. L. Muhlstein¹; E. A. Stach²; *R. O. Ritchie*¹; ¹University of California-Berkeley, Matls. Sci. & Eng., Berkeley, CA 94720 USA; ²Lawrence Berkeley National Laboratory, Natl. Ctr. for Electron Microscopy, Berkeley, CA 94720 USA

Fracture and fatigue resistance of brittle, silicon-based, structural films are important properties for the design and long-term durability of micromechanical components, especially MEMS devices. Recent work has established that such thin, micron-scale, films of single- and ploy-crystalline silicon are susceptible to premature failure under cyclic loading conditions, with failure occurring at long lives at approximately one half of the single-cycle fracture strength. However, the mechanism(s) of such failures have been a mystery. In this presentation, we propose a mechanism for the fatigue of thin-film LPCVD polysilicon based on extensive stress-life fatigue testing and high voltage transmission electron microscopy. It is proposed that the fatigue process is "surface dominated" and involves the mechanically-induced thickening of the oxide film, followed by environmentally-assisted subcritical cracking of the thickened film. Indeed, procedures, e.g., monolayer coatings, to exclude moisture and oxygen from the silicon surface are an effective means to suppress the susceptibility to fatigue failure in these materials.

9:00 AM

The Effects of Cyclic Loading on the Deformation and Fracture of Metal-Oxide Multilayers using Nanoindentation: Christy L. Woodcock¹; David F. Bahr¹; Neville R. Moody²; ¹Washington State University, Mechl. & Matls. Eng., PO Box 642920, Pullman, WA 99164-2920 USA; ²Sandia National Laboratories, Livermore, CA 94551-0969 USA

Thin metal and oxide films play an important part in the rapidly expanding microelectronics industry. In particular, the system of films with a "hard-soft-hard" gradient is vital to new microelectromechanical systems (MEMS). In this study, systems of TiO2/Ti/Si, and Al2O3/Al/ SiO2 were chosen as models for two film/substrate systems. Properties of these films are measured using nanoindentation methods with both an unloading analysis and the continuous stiffness technique. The continuous stiffness technique generates a "pop in" event during loading which is not present in monotonically loaded samples. The constant displacement oscillation value is shown to have a large impact on the frequency and peak load of these oxide excursions. Controlling the amplitude of cyclic loading from between 3 nm to 9 nm generates pop in events at decreasing loads as the amplitude is increased. Atomic force microscopy is used to show this does not appear to cause through thickness film fracture events. The possibility of interfacial failure and substrate cracking are discussed in light of the lack of exposed cracks on the surface. In addition, a finite element analysis (FEA) is used in conjunction with nanoindentation to model the depth dependent properties in materials that exhibit this same hardness gradient.

9:20 AM

Fracture of Electrodeposited Multilayered Ni/Cu Composites: *Fereshteh Ebrahimi*¹; Alirio J. Liscano¹; ¹University of Florida, Matls. Sci. & Eng., PO Box 116400, Gainesville, FL 32611 USA

Thick (20 to 40 micrometer) films of nanolayered Ni/Cu composites were produced using the electrodeposition technique. The strength and fracture behavior of free-standing films were evaluated by testing dog-bone shaped samples in tension. X-ray diffraction, transmission electron microscopy and scanning electron microscopy were employed to characterize the growth mechanism and microstructure of the multilayers. The results of this study suggest that the fracture behavior, and hence the strength, of nanolayered Ni/Cu composites is influenced significantly by the microstructure. Compatible deformation of the nickel and copper layers in samples with flat layers parallel to {100} planes resulted in knife-edge type fracture behavior. Incompatible deformation in samples with incoherent Ni/Cu interfaces parallel to {100} planes led to delamination and brittle fracture. Twining caused zig-zag growth of non-coherent layers which also resulted in constrained plastic deformation and brittle-like fracture. Development of pores during the deposition process significantly reduced the strength of the deposits.

9:40 AM

AE Monitoring of Contact Induced Plasticity and Fracture in Ultra-Small Volumes: *Natalia Tymiak*¹; Antanas Daugela¹; Thomas Wyrobek¹; William W. Gerberich²; ¹Hysitron, Inc., 5251 W. 73rd St., Minneapolis, MN 55439 USA; ²University of Minnesota, CEMS, 421 Washington Ave. S.E., Minneapolis, MN USA

Present study evaluates plasticity and fracture in ultra-small volumes utilizing Acoustic Emission (AE) monitored nanoindentation. Recently developed AE sensor integrated into an indenter tip provided a greatly enhanced sensitivity to contact loading induced transient processes and eliminated sample size effects. This enabled detection of AE events for the ultra-light contacts below 1 mN and provided an adequate basis for the AE signal analysis. Evaluations involved thin films ranging from several nanometers thick native oxides on metals to 100 nm thick SiC films on Si. Evaluated phenomena included cohesive film fracture, film/substrate delamination and yield initiation in oxidized metal surfaces. Indentation curves and in-situ images of the indented areas were correlated with the AE waveforms. Advanced procedures of AE signal decomposition provided additional information on separation of plasticity and fracture induced contributions of AE signals.

10:00 AM Break

10:20 AM

Stick-Slip Behavior of Polymer/Oxide Interfaces under Four-Point Bending: *Yvete Toivola*¹; Mat Ivill²; Brian Somerday²; Neville R. Moody²; ¹University of Minnesota, Chem. Eng. & Matls. Sci., 151 Amundson Hall, Box 128, 421 Washington Ave. S.E., Minneapolis, MN 55455 USA; ²Sandia National Laboratories, PO Box 969, Livermore, CA 94550-0969 USA

This presentation focuses on the adhesion of interfaces analogous to those encountered during MEMS component fabrication using LIGA. These metal/metal-oxide/polymer interfaces are studied using fourpoint bend sandwich test specimens. After interfacial crack initiation, the observed load-displacement (P-d) response, under displacement control, is dominated by stick-slip behavior arising from cycles of crack initiation, propagation and arrest. The origin of this stick-slip behavior was investigated through a study in which, prior to testing, sandwich specimens were exposed for seven days to a controlled temperature (either 23 or 65° C) and humidity (either dry or immersed in water) environment. Results indicated that moisture played a role in the P-d response while elevated temperatures only served to aid water diffusion through the interface. The stick-slip P-d response was repeatable over three-orders of magnitude variation in the imposed displacement rate from 2.5*10-5 to 2.5*10-3 mm/s.

10:40 AM

Macro Stress Mapping on Thin Film Buckling: *Philippe Goudeau*¹; Pascale Villain¹; Nobumichi Tamura²; ¹University of Poitiers-CNRS, LMP, UMR 6630, SP2MI, Blvd. Marie et Pierre Curie, BP 30179, Futuroscope, Chasseneuil, Vienne 86962 France; ²LBNL, ALS, 1 Cyclotron Rd., MS 2-400, Berkeley, CA 94270 USA

Thin films elaborated by sputtering techniques generally exhibit large residual stresses which may be responsible of spontaneous detachment of the film from the substrate and in the case of compressive stresses, thin film buckling. Although these effects are undesirable for future applications, one may take benefit of it for thin film mechanical properties investigation. Since 1980, a lot of theoretical works have been done to develop mechanical models with the aim to get a better understanding of driven mechanisms giving rise to this phenomenon and thus to propose solutions to avoid such problems. Nevertheless, only a few experimental works have been done on this subject to support these theoretical results and nothing concerning local stress measurement mainly because of the small dimension of the buckling. In this communication, we present micro beam x-ray diffraction measurements which have been done on 3rd generation synchrotron radiation sources for stress/strain mapping analysis of thin film buckling.

11:00 AM

In-Situ Acoustic Emission Monitoring of Nanoindentation: *Antanas Daugela*¹; Natalia I. Tymiak¹; Thomas J. Wyrobek¹; ¹Hysitron, Inc., R&D, 5251 W. 73rd St., Minneapolis, MN 55439 USA

A newly developed in-situ Acoustic Emission (AE) monitoring technique is a synergy of high bandwidth nanoscale contact characterization and advanced digital signal processing algorithms. The technique targets brittle films and substrates. High speed elastic and Surface Acoustic Wave (SAW) propagation phenomena are monitored simultaneously with quasi-static loading, by means of an AE sensor integrated into the nanoindentation test instrument. Nanometer scale contact wave propagation phenomena is observed starting from a few hundred kHz to several MHz. Advanced signal processing is an essential feature of the newly developed technique. Digital wavelet transforms and joint timefrequency analyses enhanced by neural network optimization are used for AE signal decomposition. Experimental results of AE based characterization of W(100), MgO and thin SiC films are presented, where interface cracking, delamination and fracture modes are differentiated by means of the statistical and digital signal processing analyses.

11:20 AM

Alloy Strengthening Effects on Adhesion of Gold Films: Neville R. Moody¹; David F. Bahr³; David P. Adams²; Megan J. Cordill³; ¹Sandia National Laboratories, PO Box 969, MS 9404, Livermore, CA 94551-0969 USA; ²Sandia National Laboratories, Albuquerque, NM 87185 USA; ³Washington State University, Mechl. & Matls. Eng., Pullman, WA 99164-2920 USA

Adhesion is a critical factor in the performance and reliability of gold-on-chromium hybrid microcircuits where diffusion of copper from attached leads during processing and service can alter the adhesive strength of gold films. As a result, we have studied the interfacial fracture of gold, gold-on-copper, and gold-copper alloy films on sapphire substrates to assess the effects of copper on hybrid microcircuit reliability. Nanoindentation showed that the hardness values and strengths of the gold and gold-on-copper films were similar but significantly less than corresponding values for the gold-copper alloy film due to solid solution strengthening. Tungsten overlayers and nanoindentation were then used to trigger delamination and blister formation in these three film systems from which fracture energies and interfacial bond strengths were obtained using mechanics-based models. The results revealed that the interfacial fracture energies for the gold-copper alloy film were four times higher than gold on copper and eight times higher than pure gold films. In this presentation, we will describe the techniques used to determine interfacial fracture properties, and use the results to show how alloy strengthening affects interfacial fracture. This work supported by USDOE Contract DE-AC04-94AL85000.

11:40 AM

Micro-Cracking in Contact Mechanics: Ismail Demir¹; ¹King Saud University, Dept. of Mechl. Eng., PO Box 800, Riyadh 11421 S. Arabia

Contact mechanics has been developed to investigate the behavior of materials to improve their wear and fatigue resistance. Moreover nano-indentation has been widely used to obtain some material properties and measure residual stresses. During contact loading and indentation process microcracking is observed as one of the failure modes. This can be seen in different forms as cone cracks, subsurface cracks or radial cracks on the surface. A fully coupled exact formulation of microcrack generation and interaction model in a half-plane is presented in the current study. Different forms of pressure distributions and friction conditions are assumed to investigate crack generation history during the indentation process. Two-dimensional and axisymmetric three-dimensional contacts are analyzed first. Stress intensity factors are monitored for each microcrack to control the failure and crack closure conditions are also taken into considerations. The modifications for a coating material on a substrate are outlined. The current analysis is kept in the frame of linear elastic fracture mechanics and further additions for nonlinear response are discussed for future studies.

Fatigue and Creep of Metal Matrix Composites: Fatigue of Metal Matrix Composites - II

Sponsored by: Structural Materials Division, Jt. Composite Materials Committee

Program Organizers: Nikhilesh Chawla, Arizona State University, Department of Chemical and Materials Engineering, Materials Science and Engineering Program, Tempe, AZ 85287-6006 USA; John J. Lewandowski, Case Western Reserve University, Department of Materials Science and Engineering, Cleveland, OH 44106 USA

Thursday AMRoom: 206February 21, 2002Location: Washington State Conv. & Trade Center

Session Chairs: Russ Chernenkoff, Ford Motor Company, Mfg. Sys. Dept., MD3135, Rm. 2022B, 2101 Village Rd., Dearborn, MI 48124 USA; Yu-Lin Shen, University of New Mexico, Dept. of Mechl. Eng., Albuquerque, NM 87131 USA

8:30 AM Keynote

Thermal Cycling and Thermal Fatigue Behavior of Metal Matrix Composites: Krishan K. Chawla¹; ¹University of Alabama at Birmingham, Dept. of Matls. Eng., BEC 254, 1530 3rd Ave. S., Birmingham, AL 35294-4461 USA

Thermal expansion mismatch between a ceramic reinforcement and a metallic matrix in a metal matrix composite can lead to thermal stresses under varying temperature conditions. Over the years we have studied the behavior of a variety of metal matrix composites under the thermal cycling conditions. In order of increasing complexity these are: composites with a single crystal matrix, polycrystalline matrix, precipitation hardenable matrix, and composites with metallic matrix that reacts with the ceramic reinforcement at high temperatures. Various modes of observed microstructural damage caused by thermal stresses include plastic deformation of the ductile matrix, void formation at the interface, and possible fracture of the ceramic reinforcement. Under certain conditions, quantitative damage parameters involving loss in stiffness and density can be used to study damage evolution as a function of thermal cycles. These parameters can also provide useful design information.

9:10 AM

The Cyclic Plastic Strain Response, Deformation and Fracture Behavior of 2009 Aluminum Alloy Metal Matrix Composite: *T. S. Srivatsan*¹; Meslet Al Hajri¹; ¹The University of Akron, Div. of Matls. Sci. & Eng., Akron, OH 44325-3903 USA

Development and emergence of discontinuously reinforced metalmatrix composites has created an inescapable need for a thorough and systematic understanding of microstructural effects on: (a) deformation (quasi-static and cyclic) and fracture characteristics, and (b) cyclic strain resistance and concomitant stress response characteristics and fatigue life. This technical presentation will focus on rationalizing, using principles of materials science and mechanics of solids, the underlying mechanisms governing cyclic strain-amplitude controlled fatigue response and fracture behavior of a silicon carbide particulate (SiCp)-reinforced 2009 aluminum alloy metal-matrix composite. The emphasis will be on understanding the synergistic influence of composite microstructure and test temperature on fatigue performance and associated failure modes. The key damage mechanisms will be elucidated and rationalized in light of the concurrent and mutually interactive influences of nature of loading (i.e. cyclic strain amplitude), response stress, and intrinsic composite microstructural effects. Material provided by: DWA Aluminum Composites (Chatsworth, CA, USA); (Program Manager: Mr. C. Smith).

9:30 AM

Fatigue Life Prediction of Titanium Matrix Composites by Substructuring Method: Zhenhai Xia¹; W. A. Curtin¹; ¹Brown University, Div. of Eng., 184 Hope St., Providence, RI 02912 USA

A three dimensional finite element model for predicting both crack growth and fiber breakage is developed and applied to predict fatigue crack growth and fatigue lives in a SiC-fiber reinforced Ti matrix composite. A substructuring technique is used in the finite element calculation, enabling to simulate fatigue crack growth in large-size composites without losing the details of the composite structure. Furthermore, a special elimination method is used to make the simulation process very efficient. The matrix fatigue crack is assumed nucleated on the first loading cycle by the formation of a crack in the reaction layer around a fiber and on the surface of the specimen. We first calculate both the matrix crack tip stress intensity factor and the local fiber stress concentrations due to the matrix crack, and then allow the crack to grow according to Paris-law model, and fibers to break due to statistics of the fibers. This process is repeated until composite failure occurs. Fiber failure preferentially occurs within the matrix crack region, where the fiber stresses are comparatively high, and composite failure occurs when the damage in this region is sufficient to drive fiber failure throughout the remainder of the composite in a fracture-like mode. At high stresses near the quasistatic tensile strength of the material, the central fiber inside the reaction layer crack fails upon the first loading and permits much faster initial growth of the matrix crack. Predictions for the low-cycle fatigue of Ti-matrix (IMI834) reinforced with SCS-6 SiC fibers compare well with available experimental data at high stresses.

9:50 AM Break

10:10 AM Invited

Thermo-Mechanical Characterization of MMCs by Mechanical Spectroscopy: *Efrain Carreño-Morelli*'; ¹University of Applied Sciences of Western Switzerland, Competence Grp. Matls. & Design, Rte. de Rawyl 47, Sion CH-1950 Switzerland

Damping capacity, stiffness and dimensional stability are important properties in MMC components, especially in applications requiring positioning accuracy in a changing thermal environment. Mechanical spectroscopy (damping, shear modulus and torsional deformation measurements as a function of temperature) allows to characterize the response of MMCs subjected to thermal cycling. A transient damping maximum, which is absent in monolithic materials, is observed during cooling. It is strongly dependent on reinforcement geometry and volumetric fraction, matrix strength, and interfacial strength. The damping level increases with the cooling rate, and decreases with the frequency and oscillation amplitude. This behavior originates in the relaxation of interface thermal stresses by micro-creep of the matrix around the reinforcements. An overview of damping behavior, shear modulus evolution and strain ratcheting of MMCs during thermal cycling will be presented. The results will be discussed in terms of the development of plastic zones in the matrix, near the metal-ceramic interfaces.

10:40 AM

Fracture and Fatigue of Bulk Metallic Glass Composites: John J. Lewandowski¹; Peravudh Lowhaphandu¹; Sergey Solv'yev¹; ¹Case Western Reserve University, Dept. Matls. Sci. & Eng., Cleveland, OH 44106 USA

The fracture and fatigue behavior of bulk metallic glass composites are being determined on bend specimens tested at temperatures ranging from -125C to 225C. The presentation will begin with a reveiw of work conducted to determine the static fracture toughness of bulk metallic glass using both notched and fatigue precracked specimens, followed by a review of the fatigue crack growth behavior of the bulk metallic glass tested at R=0.1 Tests conducted on toughened bulk metallic glass containing a dispersion of a crystalline metallic toughening phase will then be presented. The effects of the toughening regions on the fracture and fatigue behaivor under the different conditions will be described. Partial support provided by DARPA-SAM, Reference Metals, and AFOSR-AASERT.

11:00 AM

Fatigue Behavior of Single Ceramic Fibers: *Matthew Kerr*¹; Jason Williams¹; Nikhilesh Chawla¹; ¹Arizona State University, Dept. of Cheml. & Matls. Eng., Tempe, AZ 85287-6006 USA

Characterizing the behavior of fibers is of great importance, regardless of whether the fiber is used in woven form or as a continuous fibrous reinforcement in a composite. In a composite, it is the fiber, of course, that typically imparts high strength and stiffness to the composite. Testing of single fibers, however, is quite problematic, particularly when the fibers are brittle and exhibit poor handling characteristics. A sophisticated microforce testing system was used to conduct single fiber testing. Reproducible and stable cyclic loads were applied to study the cyclic fatigue behavior of single fibers. The elastic modulus, fiber strength (characterized by a Weibull distribution), and stress versus cycles behavior of several high performance ceramic fibers were determined. The effect of processing-induced flaws and the effect of fiber microstructure on mechanical behavior will be discussed.

11:20 AM

Fatigue Property Evaluation of Thixoformed SiCp/AZ91D Magnesium Composites: Shae K. Kim¹; Young-Jig Kim¹; ¹Sungkyunkwan University, Sch. of Metall. & Matl. Eng., 300 Chunchun-dong, Jangangu, Suwon, Gyeonggi-do 440-746 Korea

Magnesium metal matrix composites are gaining increased importance for transport and electronics applications where low inertia is required, with their improved stiffness, wear resistance, and elevatedtemperature properties. Although the use of ceramic particulate instead of fibrous reinforcements has help to reduce the over-all material cost, however, the processing-related cost should also be considered. A novel low cost Rotation-Cylinder method has been developed for preparation of particulate reinforced MMC materials, with the aim of rapid incorporation and homogeneous distribution of reinforcement particulates in an ambient atmosphere. RCM claims to significantly reduce the time required for incorporation and particulate agglomerations by the U-shaped melt surface with the Rankine vortex. Sound magnesium composites can be produced in conjunction with subsequent investment casting or thixoforming. This paper presents the results of the fatigue and wear properties of these cost effective SiCp/AZ91D magnesium composites, which were prepared by RCM and then subsequently processed by thixoforming.

Fundamentals of Advanced Materials for Energy Conversion: Complex Hydrides II

Sponsored by: Extraction & Processing Division, Process Fundamentals Committee

Program Organizers: Renato G. Bautista, University of Nevada-Reno, Department of Chemical and Metal Engineering, Reno, NV 89557-0136 USA; Dhanesh Chandra, University of Nevada-Reno, Metallurgical & Materials Engineering, Reno, NV 89557 USA

 Thursday AM
 Room: 613

 February 21, 2002
 Location: Washington State Conv. & Trade Center

Session Chairs: George Louis Powell, Y-12 National Security Complex, BWXT-Y12, LLC, PO Box 2009, Bear Creek Rd., Oak Ridge, TN 37831-8096 USA; James (Jim) E. Klein, Westinghouse Savannah River Company, Savannah River Tech. Ctr., Bldg. 773-A, Aiken, SC 29808 USA

8:30 AM Invited

The Hydriding Kinetics of Organic Hydrogen Getters: George Louis Powell¹; ¹BWXT-Y12, LLC, Y-12 Natl. Security Complex, PO Box 2009, Bear Creek Rd., Oak Ridge, TN 37831-8096 USA

The aging of hermetically sealed systems is often accompanied by the gradual production of hydrogen gas that is a result of the decay of environmental gases and the degradation of organic materials. In particular, the oxygen, water, hydrogen "equilibrium" is affected by the removal of oxygen due the oxidation of metals and organic materials. This shift of the above "equilibrium" towards the formation of hydrogen gas, particularly in crevices, may eventually reach an explosive level of hydrogen gas or degrade metals by hydriding them. The latter process is generally delayed until the oxidizing species are significantly reduced. Organic hydrogen getters introduced by Allied Signal Aerospace Company, Kansas City Division have proven to be a very effective means of preventing hydrogen gas accumulation in sealed containers. These getters are relatively unaffected by air and environmental gases. They can be packaged in a variety of ways to fit particular needs such as porous pellets, fine or coarse [gravel] powder, or loaded into silicone rubber. The hydrogen gettering reactions are extremely irreversible since the hydrogen gas is converted into an organic hydrocarbon. These getters are based on the palladium-catalyzed hydrogenation of triple bonds to double and then single bonds in aromatic aryl compounds. DEB (1,4 bis (phenyl ethynyl) benzene) typically mixed with 25% by weight carbon with palladium (1% by weight of carbon) is one of the newest and best of these organic hydrogen getters. The reaction mechanisms are complex involving solid state reaction with a herteogeneous catalyst leading to the many intermediates, including mixed alkyl and aryl hydrocarbons with the possibilities of many isomers. The kinetics of the reaction as a function of hydrogen pressure, stoichiometry, and temperature for hydrogen and deuterium near ambient temperature for pressures near or below 100 Pa over a wide range (in some cases, the complete) hydrogenation range. *Managed by BWXT Y-12, LLC for the US Department of Energy under contract DE-AC05-00OR22800.

8:55 AM Plenary

Hydrogen-Solid Interaction to Store Energy for Mobility: Louis Schlapbach¹; Andreas Züttel²; Christophe Emmenegger²; Philipp Mauron²; Patrick Sudan²; ¹EMPA-Swiss Federal Lab for Materials, Research and Testing, Dübendorf 8600 Switzerland; ²University of Fribourg, Phys. Dept., CH-1700 Friburg Switzerland

Mobility is a socioeconomic reality for which we spend about one third of our energy consumption producing significant amounts of CO2. Hydrogen, when produced from water and a clean primary energy is an attractive synthetic fuel with a high ratio of chemical energy to mass. As hydrogen is a molecular gas at room temperature compacting is an issue. High strength composite containers mechanically allow pressures up to 500bar, however, the gas-surface interaction has to be taken into account. Liquifaction goes across ortho-para conversion at a solid surface. The interaction of gaseous hydrogen with nanostructured graphitic carbon leeds to physisorption (too weak for room temperature storage) or to the formation of stable hydrocarbons. There is no clear evidence for an intermediate state. It turns out that hydrogen sorption into crystalline and amorphous metals with the formation of hydrides is a practicable and safe solution, so far limited to below 5 mass % when operated near room temperature. Several light weight metal systems, well known to form to stable hydrides of high capacity, look now more attractive due to improved catalyzed kinetics.

9:20 AM Invited

Modern Neutron Methods for the Study: John J. Rush¹; T. J. Udovic¹; ¹National Institute Standards & Technology, Ctr. for Neutron Rsrch., 100 Bureau Dr., Stop 8562, Gaithersburg, MD 20899-8562 USA

Neutron scattering and analysis techniques are extremely powerful, often unique, probes for the study of the location, bonding states and diffusion of hydrogen in all classes of materials. Developments over the past decade at NIST and elsewhere have greatly increased the sensitivity and dynamic range of neutron methods. We will review these developments and the latest state-of-the art capabilities, and provide examples of recent applications in the study of hydrogen in a number of technologically interesting systems, including metal hydrides, fuel cell materials, fullerness and carbon nanotubes, and zeolites. Examples will include measurements of dynamic behavior and vibrational spectra over a time regime from 10-8 to 10-14s.

9:45 AM

Thermal Cycling of Cold-Worked V-0.5 at.%C Alloy for Hydrogen Storage: *Dhanesh Chandra*¹; Archana Sharma¹; William N. Cathey¹; Robert C. Bowman²; Franklin Lynch³; ¹University of Nevada-Reno, Metlgel. & Matls. Eng., Mackay Sch. of Mines, MS 388, Reno, NV 89557 USA; ²NASA Jet Propulsion Laboratory, MS 79-24, Pasadena, CA 91109 USA; ³Hydrogen Consultants, Inc., 12400 Dumont Way, Denver, CO 80125 USA

The effects of thermal cycling and cold-work of V-0.5 at.%C alloy on the thermodynamic and structural parameters were investigated. Thermal cycling between β and γ phase hydrides increased the hysteresis but the desorption pressure did not significantly change. Prestraining this alloy also increased the hysteresis but the desorption pressure decreased slightly as compared to that of the unstrained alloy. Microstrains, $<\epsilon^2>^{1/2}$, in the β phase of the thermally cycled hydrides decreased after 778 cycles and the domain sizes increased. However in the γ phase, both the microstrains and the domain sizes decreased after thermal cycling. The dehydrogenated a phase after 778 thermal cycles, obtained by heating the hydrides in a differential thermal analyzer, showed residual microstrain in the lattice, similar those observed for the intermetallic hydrides. The effects of thermal cycling and cold-work on absorption and desorption pressures, H/M ratio, microstrains, long range strains and domai n sizes in the β and γ phase hydrides of V-0.5 at.%C alloy are presented.

10:10 AM Invited

Engineering Properties of Complex Hydrides: George J. Thomas¹; Gary C. Sandrock²; Karl J. Gross²; ¹University of Nevada-Reno, 537 Spirit Ridge Ct., Reno, NV 89511 USA; ²Sandia National Laboratories, Livermore, CA 94550 USA

The complex hydrides, NaAlH4 and Na3AlH6, have demonstrated rapid and reversible hydrogen storage when doped with Ti and other catalysts. These materials exhibit much greater intrinsic storage capacities, by weight, than intermetallic hydrides and have better thermodynamic properties (e.g, higher equilibrium pressures at lower temperatures) than light weight covalent hydrides. However, little is known concerning the engineering of hydrogen storage beds using these new materials. We have investigated the properties of these, as well as other related materials, which are important for their use in engineering applications. Specifically, determinations of packed bed properties, including hydrogen absorption and desorption kinetics, thermal conductivity, packing density and expansion/contraction behavior have been made. These results will be presented and discussed in terms of hydrogen storage applications.

10:35 AM Break

10:45 AM

Synthesis of Nanocrystalline Metal Hydrides by High Temperature Milling: *Jacques Huot*¹; Robert Schulz¹; ¹Hydro-Quebec, 1790 Boul. Lionel-Boulet, Varennes, Quebec J3X 1S1 Canada

It has recently been shown that magnesium-based metal hydrides such as Mg2Ni could be synthesized by high energy mechanical alloying. This process creates a nanocrystalline alloy that have enhanced hydrogen sorption properties due to the high density of defects and grain boundaries. Unfortunately, this process also requires a long synthesis time (up to 100 hours in some cases). In order to reduce processing time and cost of synthesis, we have investigated the effect of milling at elevated temperature under an inert atmosphere. Milling at high temperature improves interdiffusion of the elements and reduces the number of structural defects such as holes, dislocations and internal strain. It was found that by milling elemental powders at 200°C, a complete synthesis of Mg2Ni could be achieved in 8 hours. The hydrogen sorption kinetics and capacity of this material are comparable to Mg2Ni synthesized at room temperature.

11:05 AM

Is Carbon Material Promising for Hydrogen Storage?: Tetsu Kiyobayashi¹; Susumu Kajita²; Atsushi Ueda¹; Hiroshi Shioyama¹; Nobuhiro Kuriyama¹; ¹National Institute of Advanced Industrial Science and Technology, Special Div. of Green Life Tech., 1-8-31 Midorigaoka, Ikeda, Osaka 563-8577 Japan; ²Matsushita Electric Works, Ltd., Elect. & Plastic Matls. Co., R&D Div., 1048, Kadoma, Osaka 571-9696 Japan

Since the intriguing claims that certain carbon materials can store a huge amount of hydrogen, we have been examining the gas phase hydrogen adsorption and desorption experiments on various materials. So far we have not been able to confirm those claims. In the course of the measurement we encountered several problems which we had to circumvent in order not to obtain erroneous result. In the present paper we will explain how we can make the gas phase adsorption and desorption measurements reliable as well as our result with using the carbon materials we produced.

11:25 AM

SAES ST909 Material Phases after Methane Cracking: James E. Klein¹; Arthur R. Jurgensen¹; ¹Westinghouse Savannah River Company, Savannah River Tech. Ctr., Bldg. 773-A, Aiken, SC 29808 USA

SAES St909 is a ZrMnFe alloy with 10 wt% aluminum as a pellet binder and is used to "crack" or getter impurities from various gas streams. Bench scale methane cracking tests were performed using a stack of ten whole pellets with feed compositions ranging from 2.5 to 100 vol% methane with helium and hydrogen carrier gases, from 600 to 800°C at 760 torr and 10 sccm. XRD analyses performed on the St909 after methane cracking tests were complicated by the number of alloys that can be formed by the Zr, Mn, Fe, Al, and carbon. XRD results showed the expected ZrC alloy, but also the formation of aluminum transition metal carbides as the carbon content and the temperature of the cracking test increased. Some Al4C3 was also found in some of the pellets.

11:45 AM

Research on New Ca-Ni Based Alloys for Hydrogen Storage: *Hiroyuki T. Takeshita*¹; Yoshiyasu Sakamoto¹; Toshio Oishi²; Nobuhiko Takeichi¹; Tetsu Kiyobayashi¹; Hideaki Tanaka¹; Nobuhiro Kuriyama¹; Hiroshi Senoh¹; ¹National Institute of Advanced Industrial Science and Technology, Special Div. of Green Life Tech., 1-8-31 Midorigaoka, Ikeda, Osaka 563-8577 Japan; ²Kansai University, Dept. of Matls. Sci. & Eng., Yamada, Suita, Osaka 564-8680 Japan

Ca-Ni based alloys were examined on structures, hydrogenation properties and the effect of additional elements on hydrogenation properties. Some of the alloys were decomposed to form a new hydride which coexisted with Ni and had a CsCl-type structure on the constituent metal atoms at high temperatures such as 673K under a hydrogen atmosphere. In order to improve the stability of the original compound, the candidates of elements which were substituted for Ca or Ni in the alloys were investigated based on Miedema's semi-empirical model and Pd was chosen as a result. The effect of Pd addition on the hydrogenation properties was examined and discussed.

Fundamentals of Advanced Materials For Energy Conversion: Gas Clathrate Hydrates

Sponsored by: Extraction & Processing Division, Process Fundamentals Committee

Program Organizers: Renato G. Bautista, University of Nevada-Reno, Department of Chemical and Metal Engineering, Reno, NV 89557-0136 USA; Dhanesh Chandra, University of Nevada-Reno, Metallurgical & Materials Engineering, Reno, NV 89557 USA

Thursday AM	Room: 614
February 21, 2002	Location: Washington State Conv. & Trade Center

Session Chairs: Claudia Rawn, Oak Ridge National Laboratory, 1 Bethel Valley Rd., Oak Ridge, TN 37831 USA; E. Dendy Sloan, Center for Hydrate Research, Cheml. Eng. Dept., Colorado School of Mines, Golden, CO 80401 USA

8:30 AM Plenary

Clathrate Hydrates as Materials: E. Dendy Sloan¹; ¹Center for Hydrate Research, Cheml. Eng. Dept., Colorado Sch. of Mines, Golden, CO 80401 USA

This address is an overview of clathrate hydrates and their properties. If we wish to quantify hydrate properties, it is vital to measure the hydrate phase, rather than the associated phases. Acceptable samples are important for three reasons: (1) sample integrity and replication provides a basis for all experimental work, (2) laboratory and pipeline hydrates are significantly different from in situ hydrates, and (3) there are at least four hydrate structures from which to discriminate. Once the sample integrity is assured, three ways of measuring hydrates crystals are: (1) microscopic means e.g. X-ray/neutron diffraction, NMR, or Raman spectroscopy, (2) mesoscopic means such as SEM, single crystal formation, and growth, (3) macroscopic means such as crystal size distribution measurements. This address concerns mostly timeindependent hydrate properties, and should provide a background for the other addresses in the hydrates session.

9:10 AM Invited

Physical and Thermodynamic Properties of Gas Clathrate Hydrates Determined by In Situ Neutron Scattering: Claudia J. Rawn¹; Bryan C. Chakoumakos¹; Camille J. Jones²; Simon L. Marshall¹; Laura A. Stern³; Susan Circone³; Stephen H. Kirby³; Brian H. Toby²; Daniel C. Dender²; Yoshinobu Ishii⁴; ¹Oak Ridge National Laboratory, Metal & Cer. Div., PO 2008, Bldg. 4515, Oak Ridge, TN 37831-6064 USA; ²National Institute of Standards & Technology, 100 Bureau Dr., MS 8562, Gaithersburg, MD 20899 USA; ³US Geological Survey; ⁴Japan Atomic Energy Research Insitute, Tokai Japan

Neutron scattering methods are being applied to determine the physical behavior of technologically and environmentally important gas clathrate hydrates as a function of temperature, pressure, and composition. To date, we have studied methane deuterohydrate (Type I), CO2 deuterate (Type I), THF deuterohydrate (Type II), and a mixed methaneethane deuterohydrate (Type II) in this way. In our Rietveld refinements, the rotationally disordered guest molecules are modeled with appropriately disordered rigid bodies, which allows the temperature dependence of the mean-square-displacement of each guest molecule to be determined. This provides a means of evaluating the positional disorder of the guest molecules within the oversized cages. These results will be applied to the assessment of the stability of clathrate hydrates in geological environments. Long-term, this work will impact the development of technology for methane recovery from natural gas hydrate deposits as well as deep-ocean sequestration of industrial waste carbon dioxide. Research sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory (ORNL), managed by UT-Battelle, LLC for the US Department of Energy under Contract No. DE-AC05-00OR22725.

9:40 AM Invited

Initial Experiments on Ocean CO2 Sequestration and the Effects of CO2 Clathrate-Hydrate Formation: Edward T. Peltzer¹; Peter G. Brewer¹; ¹Monterey Bay Aquarium Research Institute, R&D, 7700 Sandholdt Rd., Moss Landing, CA 95039-9644 USA

Sequesteration of CO2 in the deep ocean as a means of reducing the atmospheric impact of fossil fuel combustion and possibly ameliorating greenhouse gas induced warming was first proposed by Marchetti (1977). A variety of ocean sequestration options have been proposed but few have been investigated beyond preliminary modeling studies or simple laboratory experiments. Through the use of MBARI's advanced ROV technology, we have begun to explore some of the ocean sequestration options. During the past five years, we have conducted a series of 7 experiments addressing some of the possible modes of ocean sequestration including mid-water releases of droplet plumes and benthic releases in deep (3000-3600 m) environments. We have observed the physical behavior of liquid CO2 in a cold, high pressure environment where clathrate hydrate formation is thermodynamically favored. Properties and processes under investigation included liquid CO2 density and buoyancy relative to the surrounding seawater, rates of dissolution of both liquid CO2 droplets and CO2 hydrate, rates of hydrate formation, effects of dissolved CO2 on pH, and the impact of CO2 sequestration on marine organisms.

10:10 AM Break

10:25 AM Invited

Dynamics of Gas Hydrates: Julian Baumert¹; Christian Gutt²; Werner Press³; John S. Tse⁴; Stefan Janssen⁵; Mark Johnson⁶; ¹Universitaet Kiel/ILL, IEAP/Compg. for Sci., 6, rue Jules Horowitz, BP 156, 38042 Grenoble France; ²Universitaet Dortmund, Experimentelle Physik I, Dortmund Germany; ³Universitaet Kiel, IEAP, Kiel Germany; ⁴NRC, Ottawa Canada; ⁵PSI, Villigen Switzerland; ⁶ILL, Grenoble France

Despite the similarities between ice and hydrates, the hydrates display some unique properties. One of the outstanding anomalies is the glass-like temperature behavior of the thermal conductivity. A main contribution to this phenomenon is thought to arise from a strong coupling between low-frequency guest and host lattice vibrations which promotes an effective scattering mechanism for the heat carrying acoustic phonons. We were able to observe the low frequency rattling modes in a high-resolution inelastic neutron experiment on Xenon hydrate [1,2]. Measured intensities point to a strong coupling which lattice dynamical calculations describe as a symmetry avoided crossing between the flat Einstein-like guest modes and the acoustic host modes. When we extended our study to methane hydrate the observed frequencies rose and the coupling mechanism changed drastically. Apparently the size and mass of the guest molecule have a strong influence on the coupling mechanism. [1] J. S. Tse, V. P. Shpakov, V. R. Belosludov, F. Trouw, Y. P. Handa, W. Press, Europhys. Lett., 54 354 (2001). [2] C. Gutt, J. Baumert, W. Press, J. S. Tse, S. Janssen, to be published.

10:55 AM Invited

Structure Characterization and Sono-Stimulated Kinetic Study with Tracers in Pressure Vessels: An Integrated Approach to the Study of Gas Hydrates: *Devinder Mahajan*¹; T. F. Koetzle¹; L. Brammer²; W. T. Klooster³; R. L. McGraw¹; R. K. McMullan¹; G. Senum¹; ¹Brookhaven National Laboratory, Tech. Dept., Chem. Dept. & Energy Scis., Upton, NY 11973 USA; ²University of Missouri-St. Louis, Dept. of Chem., St. Louis, MO 63121 USA; ³ANSTO, Lucas Heights, NSW Australia

We are using an integrated approach to study the structure and decomposition kinetics of gas hydrates. First, neutron and X-ray diffraction studies are being carried out on laboratory prepared single crystals. Building upon our earlier work including neutron and X-ray studies of the cubic II systems, 3.5Xe.8CCl4.136D2O and xH2S.8CS2.136H2O, and the unusual tetragonal bromine hydrate 20Br2.172D2O, we initially plan to study deuterated methane hydrate. This study will provide the ability to accurately characterize the hydrogen-bonded clathrate water-cage structures, including the hydrogen (deuterium) atoms and their attendant disorder. Second, two powerful techniques, sonolysis and perfluorocarbon tracers (PFTs) will be combined to conduct a kinetic study that is realistic for direct subsurface application. This study will involve methane hydrate formation in the presence of a tracer of appropriate size, followed by sono-stimulation of localized hydrate crystals in which PFT will be tracked without thermal perturbation of the surroundings. The proposed studies will be conducted in an integrated Bench-Scale Gas-Hydrate Kinetic Unit that we have specially modified for this purpose.

11:25 AM Invited

Methane and Carbon Dioxide Hydrate Investigations Utilizing a 70 Liter Pressure Vessel: *Tommy J. Phelps*¹; Olivia R. West¹; ¹Oak Ridge National Laboratory, Environmental Scis. Div., POB 2008-6036, Oak Ridge, TN 37831-6036 USA

The Seafloor Process Simulator (SPS) is a 72 liter pressure vessel developed to investigate physical and biogeochemical processes affecting the formation, stability and dissociation of methane and carbon dioxide hydrates. The vessel is 31 cm in diameter and 91 cm long containing 41 ports. The size of the SPS enables upscaling and visualizations of processes under controlled experiments. Nucleation and dissociation conditions for methane hydrates revealed that 200 mg/ liter suspensions of bentonite clays in water lowered observed nucle-

ation overpressures ~50%, corresponding to 6° of subcooling. Suspensions of silica powder lowered temperatures observed for the dissociation equilibrium ~1°. Experiments with carbon dioxide revealed dense hydrate-containing rods that sank within the SPS. Accordingly, the SPS has demonstrated usefulness for examining kinetics, formation, stability, and dissociation characteristics under controlled conditions. Importantly, upscaling of processes such as the sequestration of carbon dioxide has been demonstrated facilitating their examination under in situ conditions.

Fundamentals of Structural Intermetallics: High Temperature Strength of TiAl

Sponsored by: ASM International: Materials Science Critical Technology Sector, Structural Materials Division, Jt. Mechanical Behavior of Materials

Program Organizers: Young-Won Kim, UES, Inc., Materials & Processing Division, Dayton, OH 45432 USA; Kwai S. Chan, Southwest Research Institute, Department of Materials Science, San Antonio, TX 78284 USA; Vijay K. Vasudevan, University of Cincinnati, Department of Materials Science and Engineering, Cincinnati, OH 45221-0012 USA

Thursday AM	Room: 615-616
February 21, 2002	Location: Washington State Conv. & Trade Center

Session Chairs: Thomas R. Bieler, Michigan State University, Dept. of Matls. Sci. & Mech., 3536 Engineering Bldg., E. Lansing, MI 48824-1226 USA; Pelagia I. Gouma, SUNY Stony Brook, Matls. Sci. & Eng., 314 Old Engineering, Stony Brook, NY 11794-2275 USA

8:30 AM Invited

Creep Behaviour of TiAl Alloys with Enhanced High-Temperature Capability: *Fritz Appel*¹; ¹GKSS Research Centre, Inst. for Matls. Rsrch., Max-Planck-Strasse, Geb 45, Geesthacht D-21502 D-21502 Germany

The paper describes an experimental study of creep processes in two-phase titanium aluminide alloys involving mechanical testing and electron microscope observations. Conventional lamellar alloys suffer from insufficient creep resistance due to diffusion assisted dislocation climb processes. There are also significant microstructural changes which give rise to a complete spheriodisation of the lamellar morphology and degrade the creep strength. In an attempt to overcome these problems a novel class of alloys with the base line composition (in at.%) Ti-45Al-(5-10)Nb was developed and subjected to precipitation hardening by carbon additions. Optimized alloys exhibit significantly improved creep resistance and structural stability at the intended service conditions. The creep behaviour of these alloys was characterized in terms of the Dorn equation by thermodynamic glide parameters and detailed electron microscope analysis of the relevant micromechanisms. The results are related to processing and technical application of the alloys.

9:00 AM

Theory of Interface Properties for Carbide Precipitates in TiAl: Roy Benedek¹; ¹Argonne National Laboratory, Bldg. 223, Argonne, IL 60439 USA

Various additions to gamma-TiAl have been investigated in recent years with the objective of improving host mechanical properties, particularly high-temperature creep. Of particular interest have been the carbide precipitates Ti3AIC (cubic perovskite), and Ti2AIC (hexagonal). Properties of the interfaces of such precipitates with the matrix influence their interaction with dislocations, and thereby affect mechanical properties. First principles calculations will be presented of properties of interfaces of the above-mentioned carbides with TiAl. Interface energies and atomic structure for the different possible interface terminations will be compared. An approximate correction to the coherent interface calculations for the effect of lattice constant mismatch will be described.

9:20 AM

Effect of Aging on Creep in K5 Gamma Alloys with/without Carbon Content: *Pelagia I. Gouma*¹; Young-Won Kim²; ¹SUNY Stony Brook, Dept. MSE, 314 Old Engineering, Stony Brook, NY 11794-2275 USA; ²UES Materials & Processes Division, Dayton, OH 45432 USA

Multicomponent gamma alloys containing increased amounts of refractory elements and/or decreased aluminum contents have shown

considerably improved creep resistance over the first generation alloys such as Ti-48Al-2Nb-2Cr and XD alloys. These improvements are considered due to solid solution hardening as well as increased volume fraction of hard alpha-2 phase especially in fully-lamellar material. K5 (Ti-46Al-2Cr-3Nb-0.2W) is one example. By adding small amounts of carbon (C) and/or carbon + silicon (C+Si) to K5 alloy fully-lamellar materials were produced with to improved the creep resistance. The resulting microstructure consists of alternating layers of gamma laths and particle arrays. This paper discusses the role of isolated particle arrays during creep deformation. Fully lamellar materials were produced from three K5 alloys (K5, K5-0.2Si, and K5-0.2Si 0.1C). The results show that the aging treatment reduced creep deformation for all alloys, however, in the increasing order, indicating that alpha-2 particles interact with dislocations.

9:40 AM

Microstructure Stability during Creep Deformation of Hard Oriented PST Crystal of TiAl: Hee Y. Kim¹; Kouichi Maruyama¹; ¹Tohoku University, Dept. of Matl. Sci., Grad. Sch. of Eng., Aobayama02, Sendai 980-8579 Japan

The hard orientation with the lamellar plates oriented parallel to compression axis were deformed at 1150K under the applied stress of 158-316MPa. Microstructural changes were examined quantitatively for PST crystal during creep deformation. The six orientation variants are present with the similar proportion, but the most frequently observed γ interface is true twin type. After the creep deformation significant microstructure changes have been recognized. These are the dissolution of α_2 lamellae, the formation of ledges at lamellar interfaces, and the globularization of lamellae. Lamellar coarsening by dissolution of γ interface was observed. The fraction of 120° rotational interface and the pseudo twin interface decreased, while the faction of true twin interface increased. The twin related γ interfaces migrated by ledge formation and growth, and the interfaces disappeared by edge migration. The 120° rotational interface migrated substantially and formed equiaxed grains. The stability of α_{γ}/γ and γ/γ interfaces during creep deformation and its effect on creep resistance were discussed. The effect of stress and strain on microstructural evolution was also investigated associated with the creep deformation behavior.

10:00 AM Invited

Effect of Twinning and Stress-Induced Phase Transformation on the Primary Creep of TiAl Intermetallic Alloys: Wei-Jun Zhang¹; Seetharama C. Deevi¹; ¹Chrysalis Technologies, Inc., Rsrch. Ctr., 7901 Whitepine Rd., Richmond, VA 23237 USA

TiAl-base alloys generally exhibit a large primary strain during creep at relatively high stress levels. The mechanisms responsible for this large primary strain are not well understood yet. In this paper, the stress dependence of primary creep strain in various TiAl alloys is analyzed through modeling of the creep strain curves using thetaconcept formula. It is found that the primary strain increases significantly with increasing stress beyond a threshold stress, sth. Analysis of the experimental data suggests that the sharp increase is due to the activation of twinning and stress-induced phase transformation (SIPT) at higher stresses. Twinning and SIPT result in a large instantaneous strain e0. The influence of alloying additions and heat treatment on the sth and e0 are discussed. Appropriate aging treatment appears to be critical for engineering application of TiAl-base alloys.

10:30 AM

Comparison of Primary Creep Behaviors at Low and High Stress Region as a Function of Fully Lamellar Morphology in P/M Ti-48Al-2W: Dong Yi Seo¹; Jonathan Beddoes¹; Linruo Zhao²; ¹Carleton University, Dept. of Mechl. & Aeros. Eng., 1125 Colonel By Dr., Ottawa, Ontario K1S 5B6 Canada; ²Institute for Aerospace Research, Natl. Rsrch. Council, Struct., Matls. & Propulsion Lab., 1500 Montreal Rd., Ottawa, Ontario K1A 0R6 Canada

This paper correlates the primary creep behaviour of a near γ -TiAl+W with different fully lamellar (FL) morphologies in two different stress states. Minimizing the total primary creep and understanding the primary creep behaviour are key for several envisaged applications.Primary creep consists of two major components-the instantaneous strain and a subsequent primary transient. The primary creep behaviour at 760°C and 140 or 276MPa of P/M TiAl+W in FL conditions is evaluated. Different FL structures are produced by two step cooling from the α phase or aging treatments.The aged condition significantly improves primary creep resistance. The contribution to primary creep of the instantaneous strain and subsequent primary transient depends on the microstructural state and can be correlated to tensile yield behaviour at 760°C. At 140MPa, slightly higher instantaneous strains are observed when lamellar interface precipitates are

present, but the opposite trend occurs at 276MPa. The deformation response such as dislocation structure, dislocation reaction with third phase precipitates, and twinning at lamellar and grain boundary regions are compared in the samples crept at the different stress conditions. The results are discussed in terms of the microstructural factors controlling primary creep deformation.

10:50 AM

Interface-Controlled Diffusional Creep in Lamellar TiAl with Refined Microstructures: Luke L. Hsiung¹; ¹Lawrence Livermore National Laboratory, Chem. & Matls. Sci., L-352, PO Box 808, Livermore, CA 94551 USA

Creep mechanisms of lamellar TiAl with refined microstructures at an intermediate temperature range (650~810°C) have been investigated. A nearly linear creep behavior (i.e. the steady-sate creep rate is nearly proportional to the applied stress) was observed under stresses below ~300 MPa. Since the operation and multiplication of lattice dislocations within constituent lamellae are very limited at a low stress level, creep mechanisms based upon glide and/or climb of lattice dislocations become insignificant, instead the mobility of interfacial dislocation arrays on lamellar interfaces becomes predominant. The mobility of interfacial dislocation arrays is primarily controlled by the impingement of lattice dislocations, and the diffusion of solute segregation in lamellar interfaces. The nearly linear creep behavior observed at low-stress regime can be rationalized by the viscous glide of preexisting interfacial dislocation arrays. It is suggested that the segregation of W to lamellar interfaces has a beneficial effect to the creep resistance of refined lamellar TiAl at the low-stress regime by decreasing the mobility of interfacial dislocations.

11:10 AM

Strengthening Mehanisms in the Ti-(40-48)Al-(0-12)Nb System: Young-Won Kim¹; Dennis M. Dimiduk²; ¹UES, Inc., Matls. & Proc. Div., 4401 Dayton-Xenia Rd., Dayton, OH 45432 USA; ²Air Force Research Laboratory, AFRL/MLLM, 2230 10th St., Ste. 1, Bldg. 655, Wright-Patterson AFB, OH 45433 USA

The strengthening mechanisms of the Nb-containing two-phase gamma TiAl alloys were studied for the compositions within the representative alloy system Ti-(40-48)Al-(0-12)Nb. Alloy materials having systematically chosen compositions were produced in arc-melted cigar forms, weighing 300 g each. These were hot-die forged into plates. Samples from forged plates were annealed at 1000°C for 192h, and the resulting microstructures consisted of uniformly distributed fine equiaxed grains of constituent phases (γ , $\alpha 2$, or B2). Through detailed microprobe composition analysis, an isothermal section of the phase boundaries for the alloy system was constructed. Compressive yield strengths were measured at RT, and were found to vary with composition. A fully-lamellar material was also produced for each alloy under fixed annealing and cooling conditions. Each FL material aged at 1000°C for 24h was compression tested for yield strength measurements. An attempt is underway to explain the strength variation based on the fractions and morphologies of phases present and the solution hardening of each constituent phase as the result of Nbpartitioning. Grain size variation with composition will also be taken into account.

11:40 AM

Beta Phase Decomposition in a Grain-Refined Creep-Resistant Titanium Aluminide Alloy: Hongwei Yang¹; Tai-Tsui Cheng¹; *Mark Aindow*¹; ¹University of Connecticut, Metall. & Matls. Eng., 97 N. Eagleville Rd., Unit 3136, Storrs, CT 06269-3136 USA

In recent work it has been shown that both the properties and the microstructural stability of lamellar TiAl-based alloys can be enhanced by heavy alloying. Alloys with compositions in the range Ti-44Al-8 (Nb,Ta,Zr,Hf)-(0-0.2)Si-(0-1)B (in at. %) were investigated and it was shown that the microstructures of these were significantly different from those of binary or 48-2-2 type alloys, with lamellar plus gamma and transformed beta regions. These differences led to significant increases in the strength, creep resistance and/or ductility of these alloys depending on composition and thermal history [1,2]. In the present study we have considered the microstructural development in one of these alloys, Ti-44Al-4Nb-4Zr-0.2Si-0.3B, in more detail. This alloy was selected as having the most promising properties of those considered in the previous work. In this paper we will present TEM data obtained from this alloy after heat-treating at 1350°C and cooling to room temperature at various rates. It will be shown that the main effect of cooling rate is upon the morphology and distribution of the decomposition products in the transformed beta regions of these microstructures. In all cases the beta phase firstly orders to B2 and then decomposes to give a mixture of B2, w and g phases depending on the cooling rate. The w phase forms from the B2 both via the usual

displacive/re-ordering mechanism, and by direct precipitation giving two distinct orientation relationships. In contrast, the transformation to the g phase occurs by discontinuous coarsening of existing g lamellae. The effect that these microstructural variations might have on the mechanical behavior of the alloys will be discussed. [1] T. T. Cheng and M. H. Loretto, Acta Mater. 46:4801 (1998). [2] T. T. Cheng, M. R. Willis and I. P. Jones, Intermetallics 7:89 (1999).

12:00 PM

Effects of Gd Addition and Lamellar Spacing on Tensile and Compressive Creep Behaviours of a Fully Lamellar Ti-44Al-1Mn-2.5Nb Alloy: Kenong Xia¹; Xiaolin Wu¹; Dan Song²; ¹University of Melbourne, Dept. of Mechl. & Mfg. Eng., Victoria 3010 Australia; ²Northeastern University, Sch. of Matls. & Metlgcl. Eng., Shenyang, Liaoning 110006 China

A quaternary Ti-44Al-1Mn-2.5Nb (at%) alloy and an equivalent alloy with 0.15 at% rare earth element Gd were prepared by casting. Following heat treatments to obtain a fully lamellar microstructure, both alloys had an average grain size of ~270 µm and lamellar spacing of the order of 0.5 µm. Different heat treatments using faster cooling produced much finer lamellar spacings of the order of 0.05 µm in both alloys. Tensile creep tests showed that with the same microstructure the secondary creep rate of the Gd-containing alloy was lower than that of the quaternary alloy, and for the same alloy the material with finer lamellar spacings exhibited a significantly lower secondary creep rate than that with coarser lamellar spacings although the steady state creep observed in the latter material disappeared in the finer spaced material. However, compressive creep tests showed that a steady state creep existed in all the materials, and although the materials with finer lamellar spacings still displayed lower creep rates the effect of Gd was not observed. The results were discussed based on TEM and SEM observations.

International Symposium on Science and Technology of Interfaces in Honor of Dr. Bhakta Rath: Grain Boundaries

Sponsored by: Structural Materials Division, ASM International: Materials Science Critical Technology Sector, Electronic, Magnetic & Photonic Materials Division, Physical Metallurgy Committee, Superconducting Materials Committee, Jt. Mechanical Behavior of Materials, Titanium Committee

Program Organizers: Sreeramamurthy Ankem, University of Maryland, Department of Material & Nuclear Engineering, College Park, MD 20742-2115 USA; I. Ovidko, Russian Academy of Sciences, Institute of Problems of Mechanical Engineering, Laboratory for Theory of Defects in Materials, St. Petersburg 199178 Russia; Chandra Pande, Naval Research Laboratory, Materials Science and Technology Division, Washington, DC 20375-5000 USA; S. Ranganathan, Indian Institute of Science, Department of Metallurgy, Bangalore 560 012 India

Thursday AM Room: 617 February 21, 2002 Location: Washington State Conv. & Trade Center

Session Chairs: Dorte Juul Jensen, Riso National Laboratory, Matls. Rsrch. Dept., Fredriksborgvej, Roskilde DK 4000 Denmark; Tadao Watanabe, Laboratory of Materials Design and Interface Engineering, Dept. of Mach. Intell. & Sys. Eng., Grad. Sch. of Eng., Tohoku University, Sendai, Japan

8:30 AM Invited

In-Situ Determination of Grain Boundary Migration during Recrystallization: Dorte Juul Jensen¹; ¹Riso National Laboratory, Matls. Rsrch. Dept., Fredriksborgvej, Roskilde DK 4000 Denmark

By a novel high energy synchrotron technique it is possible to determine the crystallographic orientation and the elastic strain of micronsized local volumes in the bulk of metal samples. This technique is referred to as 3D x-ray diffraction (3DXRD) microscopy, and it has been used to follow the growth of individual grains in-situ during recrystallization. It has been found that the grains could be detected already when they were about 1µm in size, i.e. the early growth of the nuclei is also observed. In total the growth of several hundred nuclei/ grains were characterized in 2 aluminium alloys. It was found that each nuclei/grain has its own growth characteristics and that the growth rates vary significantly in time. Based on the data growth rate distributions are deduced. In the presentation, the 3DXRD microscope and the experimental procedure is shortly described. The results are summerized and discussed with reference to earlier growth rate determinations using more traditional techniques. Finally the implications of a growth rate distribution on recrystallization modelling is discussed.

8:55 AM Invited

Grain Boundary Engineering under External Fields: Tadao Watanabe¹; ¹Laboratory of Materials Design and Interface Engineering, Dept. of Mach. Intell. & Sys. Eng., Grad. Sch. of Eng., Tohoku University, Sendai Japan

Grain boundaries are important microstructural elements which can produce a wide variety of functions and also bring about a drastic improvement of performance of structural and functional polycrystalline materials. Since the concept of grain boundary design and control for high performance polycrystalline materials was proposed by the author, the concept has been widely tested and proved to be powerful for designing and developing high performance polycrystalline engineering materials, not only metallic, also ceramic and semiconductor materials, through the control of new microstructural parameters associated with grain boundaries; "Grain Boundary Character Distribution GBCD", "Grain Boundary Connectivity" and grain Boundary geometrical configurations. The present paper will discuss the ways in which grain boundaries can be effectively manipulated during processings under external fields, e.g. magnetic field, stress field, and temperature gradient, on the basis of recent investigations made by the author's group and others. High performance magnetostrictive ferromagnetic material for micromachines such as actuator and high performance photovoltaic material like polysilicon for solar cell, have been developed. I believe that it is the right time when materials scientists and engineers should recognize and utilize the importance, variety and potential of grain (including interphase) boundaries in development of high performance advanced materials even nanocrystalline materials with a huge density of boundaries, in the 21st century.

9:20 AM Invited

Atomistic Aspects of Grain Boundary Fracture: Diana Farkas¹; ¹Virginia Tech, Dept. of Matls. Sci., Blacksburg, VA 24060 USA

These studies use interatomic potentials and molecular level simulations to investigate the detailed atomistic nature of the fracture mechanisms along interfaces in metals and alloys. The many body interatomic potentials (of the embedded atom type) used for the calculations are obtained from the perfect lattice experimental properties and from first principle quantum mechanical calculations. Mixed potentials are created to describe the experimental thermodynamics of the system. Large-scale simulations of cracked bi-crystals allow the study of the fracture processes in these alloys. Dislocation emission from the crack tip and/or crack propagation are observed, and correlated with the ductile/brittle response. The role of the detailed atomistic structure of the grain boundary was found to be essential in brittle crack propagation along the interface.

9:45 AM Invited

Characterization of Grain Boundaries in the Five Dimensional Space of Mesoscopically Observable Parameters: Gregory S. Rohrer¹; David M. Saylor¹; Adam Morawiec²; Kevin W. Cherry¹; F. H. Rogan¹; Anthony D. Rollett¹; ¹Carnegie Mellon University, MSE, 5000 Forbes Ave., Pittsburgh, PA 15213-3890 USA; ²Instytut Metalurgii i Inzynierii, Materialowej PAN, Reymonta 25, 30-059, Krakow Poland

The character of a grain boundary can be determined by five mesoscopically observable parameters: three that describe the lattice misorientation and two that describe the boundary inclination. While the distribution of lattice misorientations is frequently derived from the analysis of planar sections, grain boundary inclinations are rarely reported for more than a handful of boundaries. We have used a combination of SEM, OIM, and serial sectioning to characterize the grain boundary network in polycrystalline MgO. All five degrees of freedom were defined for 7x106 square microns of grain boundary surface area in 1 cubic millimeter of the sample. We have found that there is a significant texture in the space of grain boundary planes (for boundaries of fixed misorientations). Peaks in the distribution suggest that "special" boundaries occur with high probability. The relative energies of the grain boundaries were reconstructed under the assumption that the grain boundary triple junctions were in local equilibrium. The relatively low energy boundaries correspond to peaks in the grain boundary distribution. However, simple geometric models involving dislocation arrays or coincident lattices do not predict that all of these boundaries should be special. In this paper, we will describe details of the distribution and energy anisotropy and advance plausible explanations for the observations.

10:10 AM

Coincidence Site Lattice Theory of Triple Junctions and Quadruple Points: Val Y. Gertsman¹; ¹Pacific Northwest National Laboratory, PO Box 999, P8-16, Richland, WA 99352 USA

The coincidence site lattice theory of grain boundaries is extended to multi-crystallite ensembles, in particular to triple junctions and quadruple points. It provides a basis for analyzing the junction structures as well as polycrystalline microstructure. Examples of application of the theory to some model microstructures are presented. Implications of the theory for the grain boundary engineering approach are discussed.

10:30 AM

Stochastic Method for the Evolution of Microstructures with Particular Reference to Grain Boundary Networks: Mukul Kumar¹; Roger W. Minich¹; James S. Stölken¹; Christopher Schuh¹; ¹Lawrence Livermore National Laboratory, 7000 E. Ave., L-356, Livermore, CA 94550 USA

Grain boundary engineering has been successfully applied to improve materials properties such as intergranular corrosion and cracking, creep, and weldability. This has been attributed to an increase in the fraction of special grain boundaries from thermomechanical processing. Our investigations, however, have led to the conclusion that the basis for these improvements is most likely to lie in the break-up of the connectivity of random boundary networks. The experimental determination of the network topology has been accompanied by a microstructure modeling effort that is derived from the percolative nature of the network. The problem of grain boundary networks, under crystallographic constraint, has been simulated using a stochastic approach that considers the probability distribution function for each boundary based on the fluctuations in strain energy and intrinsic characteristics such as interfacial energy. The influence of both multiplicative and additive fluctuations toward microstructural evolution during recrystallization and grain growth will be elaborated. Experimentally quantified microstructures using grain boundary character and triple junction distributions will be compared to those obtained from simulations.

10:50 AM

Clustering, Agglomeration, Pushing and Engulfment of Inclusions at High Temperature Metallurgical Melt Interfaces: Sridhar Seetharaman¹; 'Carnegie Mellon University, Dept. of Matls. Sci. & Eng., Pittsburgh, PA 15213 USA

Recent results obtained with a High Temperature Confocal Scanning Laser Microscope to visualize interfaces between molten metals and slags and advancing solidification fronts are presented. Especially, the behavior of inclusions is elucidated with respect to (i) clustering, agglomeration and separation at slag/metal interfaces and (ii) particle pushing/engulfment at solidification fronts.

Magnesium Technology 2002: Magnesium Corrosion and General Sessions

Sponsored by: Light Metals Division, Magnesium Committee, International Magnesium Association

Program Organizers: Howard I. Kaplan, Magnesium Corporation of America, Salt Lake City, UT 84116 USA; Menachem Bamberger, Technion, Israel Institute of Technology, Haifa 32000 Israel; Byron B. Clow, International Magnesium Association, McLean, VA 22101 USA; Gerald S. Cole, Ford Motor Company, Ford Research Laboratories, Dearborn, MI 48121 USA; Rod Esdale; John N. Hryn, Argonne National Laboratory, Argonne, IL 60439-4815 USA; Zi-Kui Liu, Pennsylvania State University, Materials Science and Engineering, University Park, PA 16082-5005 USA; John L. Mihelich, Metal Experts International, Winston, GA 30187 USA; Ramaswami Neelameggham, Magnesium Corporation of America, Salt Lake City, UT 84116 USA; Eric A. Nyberg, Pacific Northwest National Laboratory, Materials Processing Group, Richland, WA 99352 USA; Mihriban O. Pekguleryuz, Noranda, Noranda Technology Centre, Pointe-Claire, Quebec H9R 1G5 Canada; Bob R. Powell, General Motor Corporation, NAO Research and Development Center, Warren, MI 48090-9055 USA; Allen Schultz, Hatch, Mississauga, Ontario L5K 2R7 Canada

Thursday AM	Room: 606
February 21, 2002	Location: Washington State Conv. & Trade Center

Session Chairs: Alan Luo, General Motors, Staff Rsrch. Eng., Matls. & Proc. Lab, General Motors R&D Ctr., MC 480-106-212, 30500 Mound Rd., Warren, MI 48090-9055 USA; Howard I. Kaplan, Magnesium Corporation of America, 238 N. 2200 W., Salt Lake City, UT 84116 USA

8:30 AM

Emerging Trends in Corrosion Protection of Magnesium Die-Castings: Jan Ivar Skar¹; Darryl Albright²; ¹Norsk Hydro Research Center, Sect. for Matls. Tech., PO Box 2560, Porsgrunn N-3907 Norway; ²Hydro Magnesium, Magnesium Mkt. Dvlp., 39209 Six Mile Rd., Ste. 200, Livonia, MI 48152 USA

Due to the improved corrosion resistance of magnesium alloys brought forward by the development of the high purity grades 20 years ago, the use of die cast magnesium components has moved towards more and more demanding applications. The corrosion resistance is sufficient so that magnesium is used in the under-body environment of vehicles without additional general corrosion protection, although special attention must be given to galvanic corrosion protection. There has recently been an increasing interest in both semi-exterior and exterior automotive parts. Since magnesium alloys are not compatible with standard automotive phosphate treatments, the parts need to be pre-coated prior to assembly. For such components, the challenges are to find efficient, environmentally friendly pre-treatments and robust coating systems that can maintain their integrity through the assembly process. The present paper reviews some of the established and newly developed methods for corrosion protection and finishing of die cast magnesium automotive parts.

9:00 AM

Corrosion and Wear Resistance of Electroless Nickel on Magnesium Alloys: George E. Shahin¹; ¹Atotech USA, 1750 Overview Dr., Rock Hill, SC 29731-2000 USA

Magnesium is the world's lightest metal with a specific gravity of 1.74. Aluminum weighs 150% more, iron and steel 400% more, copper and nickel alloys 500% more and some glass filled plastic weigh 25% more. This lightness combined with a good strength-to-weight ratio of magnesium has found increasing utilization in the transportation and electronic fields. Magnesium is also the most electrochemically active metal. This high reactivity of magnesium limits its application to certain environments. This paper will discuss the pretreatment of magnesium alloys in addition to electroless nickel plating magnesium alloys. Also discussed will be the corrosion resistance of magnesium alloys nickel on magnesium alloys. The corrosion resistance will be evaluated by neutral salt spray and various electrochemical techniques.

9:20 AM

A Novel Technique to Evaluate the Corrosion Behavior of Magnesium Alloys: Basant L. Tiwari¹; John J. Bommarito¹; ¹General Motors, R&D Ctr., Matls. & Proc. Lab., MC 480-106-212, Warren, MI 48090-9055 USA

A novel technique for measuring the intrinsic corrosion rate of magnesium alloys has been developed. As a magnesium alloy sample dissolves in 5% NaCl solution, the dissolution rate is determined by measuring the amount of HCl added to the NaCl solution to control the pH between 5 and 7. The corrosion rate is determined from the slope of the curve where the dissolution rate reaches a steady state. The technique was used to compare the corrosion behavior of newly developed creep-resistant magnesium alloys with several known magnesium alloys. It was shown that the corrosion rate of AC52 (Mg-5%Al-2%Ca) is comparable to AZ91D. This technique provides a fast way to screen the effect of small composition changes on corrosion behavior of Mg alloys. Because of the short test time, this technique provides a powerful tool to accelerate alloy and product development with Mg alloys.

9:40 AM

Aqueous Corrosion Characteristics of Mg-4Ni-xAl Alloys in Acid-Chloride Solution: *Yoon-Seok Choi*¹; Jung-Gu Kim¹; Shae K. Kim¹; Young-Jig Kim¹; ¹School of Metallurgy & Material Engineering, 300 Chunchun-dong, Jangan-gu, Suwon, Gyeonggi-do 440-746 Korea

Aqueous corrosion properties of Mg-4Ni-xAl alloys in acid-chloride solution were studied. Three NA40, NA41 and NA42 alloys were prepared by Rotation-Cylinder Method. The corrosion behavior of them was investigated at room temperature by polarization tests, pH measurement, hydrogen evolution test, galvanic corrosion tests and surface analyses. The results of polarization test indicated that with increasing Al content, (a) the corrosion potential had more active potential while corrosion rate decreased and (b) the segregation of the á-Mg/Mg2Ni eutectic phase at grain boundary was reduced. This is because micro-galvanic reactions (a) between the Mg matrix and the á-Mg/Mg2Ni eutectic phases and (b) between the á-Mg and Mg2Ni in the eutectic phase itself were reduced, which decreased the corrosion rate of Mg alloys. Galvanic corrosion tests for consideration of Mg-4NixAl alloys as structural materials were also done compared to AZ91D Mg alloy coupled with low carbon steel, Al alloy and Cu alloy.

10:00 AM

Improved Corrosion Performance of AZ91D Magnesium Alloy by the KeroniteÔ Coating Process: S. Shrestha¹; A. Sturgeon¹; P. Shashkov²; A. Shatrov²; ¹TWI, Ltd., Granta Park, Great Abington, Cambridge CB1 6AL UK; ²Keronite, Ltd., PO Box 700, Granta Park, Great Abington, Cambridge CB1 6ZY UK

This paper describes the results of a study on the corrosion behaviour of a die cast magnesium alloy type AZ91D coated with the KeroniteÔ process. This process is a new commercially available and environmentally friendly electrolytic coating method applicable to all types of magnesium alloys. The process involves creation of a hard ceramic oxide layer onto a light substrate alloy by plasma electrolytic oxidation (PEO) in a low concentrated alkaline solution. Corrosion performances were assessed in a 3.5% NaCl solution using an accelerated electrochemical potentiodynamic polarisation method (ASTM G61) and a 1000-hour of salt spray exposure (ASTM B117). Galvanic corrosion tests were performance, parallel tests were carried out on an uncoated AZ91D alloy. The study demonstrated the improved corrosion resistance of Keronite coated AZ91D magnesium alloy and its potential for use in severe corrosive environments.

10:20 AM Break

10:35 AM

Sealing Methods for Enhanced Corrosion Protection of Anodized Magnesium Alloy WE43A-T6: *Richard George Rateick*¹; Shen-Jiang Xia²; Viola I. Birss²; ¹Honeywell International, Engines & Sys., 717 N. Bendix Dr., S. Bend, IN 46637 USA; ²University of Calgary, Chem. Dept., 2500 University Dr. N.W., Calgary, Alberta T2N 1N4 Canada

High voltage anodizing processes continue to be developed for providing corrosion protection to magnesium alloys. However, the large pore structure in these coatings represents a barrier to further increases in corrosion resistance. The objectives for the work reported here were to develop methods of sealing the pores in complex parts where reentrant surfaces preclude the use of spray type top coating systems. A second objective was that the coating not flake off of internal surfaces, thus eliminating a source of foreign object damage for aerospace applications. Salt fog, electrochemical impedance, throwing power and adhesion data will be presented for anodized magnesium alloy WE43A-T6. The anodization was performed using both a commercial and a developmental process. The sealing operations were performed using Parylene grades C and HT. The Parylenes are vapor deposited polymers.

10:55 AM

Joining of Light Hybrid Constructions Made of Magnesium and Aluminum Alloys: Adi Ben-Artzy¹; Avraham Munitz²; Gavri Cohn¹; Avigdor Shtechman¹; ¹Rotem Industries, Ltd., Metal Forming Grp., POB 9046, Beer-Sheva 84190 Isreal; ²N.R.C.N, POB 9001, Beer-Sheva 84190 Isreal

Magnesium alloys are widely used in automotive applications due to reduction in fuel consumption and to their good energy absorption. The growing demand for improved mechanical properties and longer fatigue life has increased the implementation of wrought magnesium alloys, especially for moving and safety parts. For some applications, joining of different magnesium alloys produced by extrusion, forging, or high-pressure die-casting, is essential to enable the manufacturing of complex parts and hybrid structures. Since magnesium alloys occupy only a small fraction of materials used for cars or aircraft construction, it is essential to join (weld) the alloys to other frames and body parts. Therefore, joining (welding) of dissimilar materials i.e. aluminum or steel alloys to magnesium alloys is essential. When highpressure die-cast alloys such as AM50 was welded to other alloys, the welding heat popped up the close porosity of the cast parts, and weakened the joint area by creating foam-like zones. It was found that use of high energy focused welding system like an electron Beam (EB) or a laser, the effect of heat on the die cast alloy is reduced, and a strong joint is formed. In the present study, Al-6063 and different magnesium alloys were EB and GTAW welded. It was found that Beta-Mg17Al12 phase is formed in the fused zone. The presence of this inter-metallic phase is the main reason causing brittleness and low strength of the joints. There are indications that use of proper welding electrode composition may reduce this problem, and eventually enable the welding of dissimilar joints of aluminum and magnesium alloys.

11:15 AM

Resistance Spot Welding of Mg AM50 and AZ91D Alloys: *Abraham Munitz*¹; C. Cotler¹; Gabrial Kohn²; ¹Nuclear Research Center-Negev, PO Box 9001, Beer Sheva 84190 Israel; ²Rotem Industries, Rotem Industrial Park, PO Box 9046, Beer Sheva 84190 Israel

Resistance spot welding of Mg AM50 and AZ91 2-mm thick castplates were successfully performed. The welds were examined by X-ray radiography, conventional optical microscopy and scanning electron microscopy. It was found that the weld nugget consisted of two regions; I) Central molten zone, II) Partially melted Heat Affected Zone (HAZ). The size and morphology of the nugget depend on 3 main factors: i) The alloy composition, i.e. circular morphology for Mg-AM50, and rectangular for Mg-AZ91D. ii) Current. i.e. the higher the current, the larger was the central melted zone. iii) Pulse duration: A minimum pulse duration of 2 s was needed for creating a bond. Above 2 s, longer current duration resulted in larger central molten zones. Under our experimental conditions, the pressure of the electrodes during welding had only a minor effect on the weld morphology. Grain boundary melting was observed in the majority of the HAZ. These created short-cut channels for melt transfer to the outer surface even far away from the central molten zone, which in turn caused depression of the surface of the welded plates, and shrinkage porosity in the nugget. The latter depended also on the porosity in the cast plates near the nugget. The impact of molten grain boundary and thermo-mechanical processing on the nugget morphology and its mechanical properties will be discussed by current solidification theories.

11:35 AM

The Study on Friction Stir Welding of AZ31 Mg Alloy: *Won Bae Lee*¹; Seung Boo Jung¹; Yun Mo Yeon²; ¹Sung Kyun Kwan University, Dept. of Adv. Matl. Eng., 300, Chun Chun Dong, Jang An Gu, Suwon, Kyung Gi Do 440-746 Korea; ²Suwon-Science College, Dept. of Automatic-Welding Eng., Whasung, Kyung Gi Do 445-742 Korea

Friction stir welding is a new, solid-state welding technique which was invented by The Welding Institute(TWI) in 1991. The recent studies have restricted to aluminum alloy so few data was published about welding of Mg alloy and other materials. Mg alloy are potential candidate to replace aluminum alloys in many structural application, due to some of their unique properties. Mg alloy have a low density, high strength-to-weight ratio and good castability. They are considered advanced materials for energy conservation and environmental pollution regulation. Joining of Mg parts, which may be crucial for these application, is still limited. Mg alloy are easily oxidized in welding zone because of high chemical reactivity at high temperature. So Mg alloy have a many weld defect by conventional fusion welding method. The purpose of this research is to evaluate the applicable possibility of FSW in AZ31 joining.

11:55 AM

Thermophysical Property Measurement of Magnesium Alloy: AE42: Deming Wang¹; R. A. Overfelt¹; Yemi Fasoyinu²; Mahi Sahoo²; ¹Auburn University, Mechl. Eng., 201 Ross Hall, Auburn, AL 36849 USA; ²CANMET/MTL, 568 Booth St., Ottawa K1A 0G1 Canada

This paper will present some methods to measure thermophysical properties of magnesium alloys in Auburn University. Such as measuring special heat, latent heat, solidus and liqudus temperatures, solid fraction in mushy zone by using the DSC technique; measuring thermal expansion and density by using the dilatometer and laser distance detection technique; measuring viscosities of these molten alloys by using the oscillating cup viscometer technique. Accurately to measure these data is very important for the computer modeling programs. The paper will discuss how to control measurement errors, reduce oxidization and some details about above employed techniques in these measurements of magnesium alloys. In addition, applications and experimental measuring data are presented in the paper for a magnesium alloy, AE42.

Phase Stability, Phase Transformations & Reactive Phase Formation in Electronic Materials - IV

Sponsored by: Electronic, Magnetic & Photonic Materials Division, Structural Materials Division, Alloy Phases Committee Program Organizers: Sinn-Wen Chen, National Tsing-Hua University, Department of Chemical Engineering, Hsinchu City 300 Taiwan; C. Robert Kao, National Central University, Department of Chemical Engineering, Chungli City, Taiwan; Hyuck Mo Lee, Korea Advanced Institute of Science & Technology, Department of Materials Science & Engineering, Taejon 305-701 Korea; Michael R. Notis, Lehigh University, Department of Materials Science, Bethlehem, PA 18015 USA; Douglas J. Swenson, Michigan Technological University, Department of Metallurgical & Materials Engineering, Houghton, MI 49931 USA

 Thursday AM
 Room: 211

 February 21, 2002
 Location: Washington State Conv. & Trade Center

Session Chairs: C. Robert Kao, National Central University, Dept. of Cheml. & Matls. Eng., Chung-li Taiwan; S. W. Chen, National Tsing-Hua University, Dept. of Chem. Eng., #101 Kuang-Fu Rd., Sec. 2, Hsin-Chu 30043 Taiwan

8:30 AM Invited

Phase Equilibria and Solidification Properties of Sn-Cu-Ni Alloys: Sinn-Wen Chen¹; Chih-Hao Lin¹; ¹National Tsing-Hua University, Cheml. Eng., 101, Sec. 2, Kuang-Fu Rd., Hsin-Chu 300 Taiwan

Ternary Sn-Cu-Ni alloys were prepared and annealed at 240°C. The annealed alloys were metallographically examined and the equilibrium phases formed were identified based on the compositional determinations and x-ray diffraction analysis. The isothermal section of the ternary Sn-Cu-Ni system at 240°C was proposed based on the experimental results of this study and related phase equilibrium knowledge in the literatures. The binary compounds, Cu6Sn5, Ni3Sn2, and Ni3Sn4 have very extensive ternary solubility. Continuous solid solutions are formed between Cu and Ni as well as between Cu3Sn and Ni3Sn. Besides the isothermal section, the liquidus projection of Sn-Cu-Ni system was determined based on previous literature results and the information of primary solidification phases of various Sn-Cu-Ni alloys examined in this study.

8:55 AM Invited

Copper Migration Phenomena in IC Package under High Temperature Aging: Hen-So Chang¹; *Ker-Chang K. Hsieh*¹; Theo Martens²; C. C. Chen²; ¹National Sun Yat-Sen University, Inst. of Matls. Sci. & Eng., Kaohsiung Taiwan; ²Philips Electronic Building Elements Industries (Taiwan), Ltd., Tech. Dev. Div., 10, Chin 5th Rd., N.E.P.Z., PO Box 35-48, Kaohsiung Taiwan

Copper migration phenomena found in several IC samples during the new materials evaluation for the IC plastic package. The copper atom can migrate from the copper leadframe through the gold wire surface and reach the ball bond. The Cu-Au alloy phase formed on the gold wire surface as well as the Cu-Au-Al alloy phase formed on the ball bond. Another phenomenon is the copper atom may react with the phosphorus particles, which used as flame retardant in green compound. Cu3P and CuP2 phases formed inside the plastic compound and cause the short circuit failure. The atom migration phenomena are due to three driving forces: diffusion, alloy formation and Galvanic effect.

9:20 AM Invited

Diffusion Soldering for High Temperature Stable Thin Film Bonds: Rainer Schmid-Fetzer¹; Thomas Studnitzky¹; ¹Technical University of Clausthal, Inst. of Metall., Robert-Koch-Str. 42, Clausthal-Zellerfeld D-38678 Germany

Diffusion soldering (DS), a special form of transient liquid phase bonding (TLP) or isothermal solidification (IS) can be used to form strong bonds at low temperature which remain solid up to a much higher remelting temperature. Thin film processing makes DS especially attractive for micro/optoelectronics or microsystems if the joined parts are exposed to higher temperature in later steps of device fabrication. In conventional DS systems, composed of (near) noble metals with Sn or In, the remelting temperatures are typically limited to around 400 to 500°C. In this work new DS systems involving also (early) transition metals with Sn are investigated, which may show much higher remelting temperatures. Phase formation and reaction kinetics of these systems were studied, they are essential for controlling the DS process.

9:45 AM Invited

Morphological Studies on IMC Formed between Nickel Particles and Sn-Ag Solder: K. N. Subramanian¹; J. Lee¹; F. Guo¹; J. P. Lucas¹; ¹Michigan State University, Dept. of Matls. Sci. & Mech., 3536 Engineering Bldg., E. Lansing, MI 48824-1226 USA

Morphology of the intermetallic compound (IMC) layer formed around mechanically-incorporated Ni particle in eutectic Sn-Ag solder under various reflow conditions was studied. Two distinct morphologies, sun-flower and faceted single crystal, were observed. Effects of heating and cooling rates on the morphological changes were investigated to identify the processing parameters that contribute to these morphologies. Results of IMC formation noted with Ni particles will be compared with those obtained with Ag and Cu particle reinforced composite solders. Acknowledgement: Project funded by Composite Materials and Structures Center at Michigan State University.

10:10 AM Break

10:30 AM

Phase Transformations and Microstructure Evolution in Cu-Ge Alloys: Sumanth Jagga²; *Vijay K. Vasudevan*¹; ¹University of Cincinnati, Dept. of Matls. Sci. & Eng., Cincinnati, OH 45221-0012 USA; ²Convergys, Inc., Cincinnati, OH 45201 USA

Alloys based on the Cu-Ge system, especially those on the ε_1 -Cu₃Ge compound, have considerable potential for application as interconnects in microelectronic devices because of their attractive electrical and barrier properties. Though the thermodynamics of this system has been assessed based on available data, knowledge of phase equilibria, structures of phases and phase transformations is far from complete. The present study was undertaken to address these aspects. Arc-melted cigars of five Cu-Ge alloys ranging in composition from 10 to 30 at.%Ge were prepared, homogenized and then subjected to a series of high temperature treatments followed by quenching in various media. Transformations and reaction temperatures were studied by DTA and the microstructures of both as-cast and heat treated samples were characterized by XRD, OM, SEM, EPMA and TEM. The kinetics and temperature dependence of transformations during continuous cooling were studied using a novel, computer-controlled in-situ temperature and electrical resistivity measurement system, coupled with postmortem analysis of the microstructures. Reaction start and finish temperatures, continuous cooling diagrams, enthalpies and driving forces associated with the $\epsilon\text{-}\epsilon_2$ to ϵ_1 phase transformation were determined for alloys containing 20 to 30 at.%Ge. New results related to the structure of the high-temperature phases and the nature of the transformation to ε_1 were obtained. These results will be presented and discussed.

10:50 AM

Interfacial Reactions between Ni/Cu UBM and Eutectic Sn-Pb Solder in Flip Chip Technology: Chien Sheng Huang¹; Yen Ming Chen²; Jenq-Gong Duh¹; ¹National Tsing Hua University, Dept. of Matls. Sci. & Eng., 101, Sec. 2 Kuang Fu Rd., Hsinchu 300 Taiwan; ²National Chiao Tung University, Dept. of Matls. Sci. & Eng., 1001 Ta Hsueh Rd., Hsinchu 300 Taiwan

Interfacial reactions between Ni/Cu under bump metallurgy (UBM) and eutectic Sn-Pb solder in the 63Sn-37Pb/Ni/Cu/Ti/Si3N4/Si multiplayer structure for the flip chip technology were investigated. The types of interfacial reaction products varied with different reflowed times. After the first reflow, the (Cu, Ni)6Sn5 IMC was found between solder and Ni. It was argued that Cu diffused through Ni during the reflow process due to the columnar structure of Ni. There were two interfacial reaction products formed between solder and UBM after three times of reflow. The layered (Ni, Cu)3Sn4 was next to the Ni/Cu UBM. The island-like (Cu, Ni)6Sn5 was formed between (Ni, Cu)3Sn4

and solder. It was also observed that part of the island-like IMC stripped into the solder. The diffusion path for solid-liquid reaction during periods of reflow could be determined with the aid of ternary Sn-Cu-Ni phase diagram.

11:10 AM

Nucleation Mechanisms of Copper during Electrodeposition of Thin Films from EDTA Solutions: *Batric Pesic*¹; Darko Grujicic¹; ¹University of Idaho, COMER, Dept. of Metlgel., Matls. Sci. & Eng., Moscow, ID 83844-3024 USA

The complexing and surface leveling properties of EDTA were studied during the nucleation of copper electrodeposition of thin films. Cyclovoltammetric (CV) and chronoamperometric (CA) electrochemical techniques were utilized in this study. Near atomically smooth glassy carbon was used as the deposition substrate. Morphological characterization was performed by atomic force microcopy. The copper nucleation mechanisms were examined as a function of solution pH, copper concentration, Cu:EDTA ratio. Electrochemical surface pretreatment effect was also examined. It was found that pH, copper concentration, surface pretreatment and the deposition voltage all had profound effects on the morphology of copper nuclei in the thin film. The CV and CA results, as a function of these parameters, will be discussed. The verification of instantaneous nucleation mechanisms will be presented.

Surface Engineering: Science & Technology - II: Characterization/Modeling

Sponsored by: Materials Processing & Manufacturing Division, Surface Engineering Committee

Program Organizers: Ashok Kumar, University of South Florida, Department of Mechanical Engineering, Tampa, FL 33620 USA; Yip-Wah Chung, Northwestern University, Department of Materials Science & Engineering, Evanston, IL 60208 USA; Gary L. Doll, The Timken Company, Canton, OH 44706 USA; D. S. Misra, Indian Institute of Technology-Bombay, Department of Physics, Powai, Mumbai 400076 India; John J. Moore, Colorado School of Mines, Department of Metallurgy and Materials Engineering, Golden, CO 80401 USA; Kryoshi Yatsui, Nagoka University of Technology, Nagaoka, Niigata 840-2188 Japan

 Thursday AM
 Room: 203

 February 21, 2002
 Location: Washington State Conv. & Trade Center

Session Chairs: D. S. Misra, Indian Institute of Technology, Powai, Mumbai 400076 India; Susan Pran Krumdieck, Dept. of Mechl. Eng., Christchurch 8004 New Zealand

8:30 AM Invited

Abrasive Wear Behaviour of Laser-Clad and Post Heat-Treated Tool Steel Coatings: *Sheng-Hui Wang*¹; Jianyin Chen¹; Lijue Xue¹; ¹National Research Council Canada, Integrated Mfg. Tech. Inst., 800 Collip Cir., London, ON N6G 4X8 Canada

A comparative study of abrasive wear behaviour has been conducted on several laser-clad and post heat-treated tool steel coatings. Multilayer cladding with comparable thickness was deposited using a CW CO2 laser in combination with blown powder technique. The abrasive wear resistance of the clad coatings was evaluated using a dry sand/ rubber wheel apparatus as per ASTM standard test method, and is compared to that of AISI D2 tool steel (60 HRC) which is often used as a reference material for evaluating abrasive wear resistance. Laserclad CPM-15V and CPM-10V coatings exhibit superior abrasive wear resistance than D2 baseline. In contrast, the wear resistance of laserclad CPM-9V and M4 coatings is inferior to that of the D2. The post heat-treatment of laser-clad coatings can either increase or decrease their wear resistance, depending on the material as well as the annealing temperature used. The wear scars of the laser-clad coatings were examined and the related wear mechanism has been elucidated in details.

8:55 AM

In Situ Nanoindentation of Thin Films in a Transmission Electron Microscope: Andrew M. Minor¹; Eric A. Stach²; J. W. Morris¹; ¹University of California, Dept. of Matls. Sci. & Eng., Matls. Scis. Div., Lawrence Berkeley Natl. Lab., One Cyclotron Rd., MS 66-200, Berkeley, CA 94720 USA; ²Lawrence Berkeley National Laboratory, Natl. Ctr. for Electron Microscopy, One Cyclotron Rd., MS 72, Berkeley, CA 94720 USA The nanomechanical behavior of small solid volumes exhibits fundamental phenomena that are obscured on coarser scales. We have developed a novel experimental technique of in situ nanoindentation of thin films in a transmission electron microscope. This technique can image in real time the discrete deformation mechanisms of nano-scale volumes, while simultaneously correlating this behavior with quantitative information. Issues to be discussed will be related to the initiation of defects at the surface, the effect of grain size and the role of grain boundaries in deformation of nano-scale volumes.

9:10 AM

Curvature Method as a Tool to Evaluate Shape Memory Effects for TiNiCu Thin Films: *Yongqing Fu*¹; Hejun Du¹; Sam Zhang¹; ¹Nanyang Technological University, Sch. of Mech. & Production Eng., 50 Nanyang Ave. 639798 Singapore

TiNi and TiNiCu films were prepared by co-sputtering of TiNi target with Cu and Ti targets. Curvature method was used to measure residual stress and evaluate shape-memory effects. Deposition at 723 K gave rise to low stress; deposition at room temperature resulted in large tensile stress that could be relaxed through post deposition annealing at 923 K. Upon heating, TiNiCu films generated large tensile stress when transforming from martensite to austenite, whereas during cooling, the stress relaxed significantly when the films transformed back to the ductile martensite phase. Both one-stage and two-stage phase transformations were observed and confirmed by DSC and XRD studies. Residual stresses were measured as a function of temperature that cast light on the SMA film's crystallization and transformation temperatures, recoverable, thermal, intrinsic and martensitic yield stresses. Effects of film thickness, heating rate, annealing process and cyclic heating/cooling process on martensite phase transformation were discussed.

9:25 AM Cancelled

Characterization of a Platinum Aluminide Coating after Isothermal and Thermocyclic Heating: *Hyungjun Kim*

9:40 AM

Nucleation Mechanisms of Copper during Electrodeposition of Thin Films: *Batric Pesic*¹; *Darko Grujicic*¹; ¹University of Idaho, Matls. Sci. & Eng., COMER-McClure Hall, Moscow, ID 83844-3024 USA

The nucleation mechanisms of copper during electrodeposition of thin films from pure copper sulfate solutions were studied by utilizing cyclovoltammetric and chronoamperometric electrochemical techniques. Near atomically smooth glassy carbon was used as the deposition substrate. Morphological characterization was performed by atomic force microscopy. The copper nucleation mechanisms were examined as a function of solution pH and copper concentration. Electrochemical surface pretreatment effect was also examined. It was found that pH, copper concentration, surface pretreatment and the deposition voltage all have important effects on the morphology of copper nuclei in the thin film. Chronoamperometric studies were utilized as a diagnostic tool for mechanisms of copper nucleation. It was found that copper nucleation was happening via instantaneous nucleation mechanisms.

9:55 AM Break

10:10 AM Invited

Synthesis of Functional Materials Utilizing Pulsed Power Technologies: K. Yatsui¹; W. Jiang¹; H. Suematsu¹; T. Suzuki¹; Y. Kinemuchi¹; S.-C. Yang¹; ¹Nagaoka University of Technology, Extreme Energy-Density Rsrch. Inst., 1603-1 Kamitomiokamachi, Nagaoka, Niigata 940-2188 Japan

We have proposed two applications of pulsed power technologies to material synthesis. One is a thin film preparation method by ion-beam evaporation (IBE) and another is a nanosize powder synthesis method by pulsed wire discharge (PWD). Preparation of various functional materials by IBE and PWD has been demonstrated. In IBE, a target is bombarded by an intense, pulsed proton beam. The ablation plasma, which forms from the target, deposits on substrates. Crystallized SrAl₂O₄:Eu,Dy, B₄C and TiFe thin films have successfully been prepared by IBE without substrate heating or sample annealing. Typical initial deposition rate is ~5 mm/s, which is almost 10⁶ times faster than those by conventional thin film preparation methods. In PWD, thin wires placed in a chamber are discharged and evaporated by charged capacitors. The vapor is cooled by and reacts with gas in the chamber. Various powders, including double oxides, have been synthesized by PWD.

10:35 AM

Surface Phenomena in Diffusion-Limited Capillary Penetration of a Porous Film by a Reactive Fluid: *Rajiv Asthana*¹; ¹University of Wisconsin-Stout, Mfg. Eng. Prog. Tech. Dept., 326 Fryklund Hall, Menomonee, WI 54751 USA

The capillary-driven penetration of a porous film by a reactive fluid is accompanied by pore shrinkage (or expansion) and contact angle decay, both of which modulate the capillary pressure driving the flow. The kinetics of diffusion-limited capillary flow of a reactive liquid in a porous film is modeled for the case of a shrinking pore and an exponentially decaying contact angle in a manner similar to the case of interface-limited flow presented elsewhere[1]. The computational outcomes for penetration of porous Si3N4 films by AgCuTi brazes, and of porous carbon films by Si confirm that, for an unstable contact angle, greater penetration is achieved at lower values of the diffusion rate constant. A classical capillary flow analysis overestimates the kinetics whereas a shrinking pore model with a constant contact angle underestimates the kinetics. The calculated limiting lengths at pore closure exhibit a better agreement with the recent measurements in the Si/C system as compared to current models of reactive flows. [1] R. Asthana, Surface Engineering in Materials Science - I, Seal, Dahotre, Moore and Mishra, eds., TMS, 2000, pp 287-297.

10:50 AM

Influence of Surface Roughness on the Coercivity and Magnetic Interactions in CoCrX (X=Pt,Pd,Ta,B) Thin Film Media: Mehmet Tarakci¹; Siva Guruswamy¹; ¹University of Utah, Metlgcl. Eng., 135 S. 1460 E., Rm. 412, Salt Lake City, UT 84112-0114 USA The influences of Al-Mg/NiP alloy disk surface roughness ranging from 2 Å to 50 Å on the morphology, coercivity and magnetic inter-Co81Cr17B2, actions in Co83Cr17, Co78.5Cr17Pt4.5, Co78.5Cr17Pd4.5, Co76.5Cr17Pt4.5B2, Co78.5Cr17Ta4.5, Co76.5Cr17Ta4.5B2, Co75.5Cr17Pt4.5Ta3, Co72Cr13Pd12Ta3 and Co84Cr10Ta6 alloy thin films on Al-Mg/NiP/Cr substrates were examined. The grain morphologies were characterized using atomic force microscopy. The samples were prepared under conditions optimized for obtaining in-plane Cr (002) orientation and Co (11-20) orientation. The coercivity and coercivity ratio of the CoCr alloy films increase with increase in the substrate surface roughness, particularly in the range below 10 Å. The magnetic interactions are strongly influenced by the circumferential substrates surface texture. Exchangecoupling decreases as the surface roughness of the substrates is decreased. Additions of Ta and Cr are effective in reducing the exchange coupling while Pt and Pd additions have an opposite effect at an addition level of 4.5 at.%.

11:05 AM

Effect of Faceting on the Thermal Grain Boundary Grooving of Tungsten: *Joachim H. Schneibel*¹; Pavlo P. Sachenko²; Wen Zhang³; ¹Oak Ridge National Laboratory, Metals & Cer. Div., PO Box 2008, Oak Ridge, TN 37831-6115 USA; ²Oakland University, Dept. of Mechl. Eng., Rochester, MI 48309 USA; ³Oakland University, Dept. of Math. & Stats., Rochester, MI 48309 USA

The grain boundary grooving of polycrystalline tungsten annealed at 1350°C was studied by atomic force microscopy. The profiles of the grooves between unfaceted grains were in qualitative agreement with the predictions of Mullins theory of grooving by surface diffusion. In particular, the predicted secondary maxima and minima next to the main groove maxima were often observed. Surface faceting strongly affected the grooving kinetics and groove shapes. In particular, the grooves developed between faceted grains often exhibited smaller ridges than those between unfaceted grains. Grooves forming between faceted and unfaceted grains were often asymmetric. The shapes of the asymmetric grooves could be numerically modeled by assuming that faceting inhibits surface diffusion. This material is based upon work supported by the National Science Foundation under grant DMR-9996087. Research at the Oak Ridge National Laboratory SHaRE User Facility was sponsored by the Division of Materials Sciences and Engineering, US Department of Energy, under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

11:20 AM Cancelled

Molecular Polarizability of Fullerene and Graphite Clusters: *Francisco Torrens*

11:35 AM

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Studies on the Structure and Characteristics of Electrodeposited RE-Ni-W-P-B4C-PTFE Composite Coatings: *Zhongcheng Guo*¹; Xiaoyun Zhu¹; ¹Kunming University of Science and Technology, Fac. of Matl. & Metall. Eng., Kunming 650093 China This paper mainly describes friction and wear characteristics of the electrodeposited RE-Ni-W-P-B4C-PTFE composite coating. It also explains the reason for these fine characteristics in view of structure.

Teaching and Learning Hydrometallurgical Science and Engineering: Educational Technology

Sponsored by: Extraction & Processing Division, Aqueous Processing Committee, Copper, Nickel, Cobalt Committee, Precious Metals Committee, Waste Treatment & Minimization Committee Program Organizers: Kwadwo Osseo-Asare, Pennsylvania State University, Metals Science and Engineering, University Park, PA 16802-5006 USA; Saskia Duyvesteyn, University of Utah, Department of Metallurgical Engineering, Salt Lake City, UT 84112-0114 USA

Thursday AM	Room: 601
February 21, 2002	Location: Washington State Conv. & Trade Center

Session Chairs: Saskia Duyvesteyn, University of Utah, Metlgcl. Eng., 135 S. 1460 E., Rm. 412, Salt Lake City, UT 84112-0114 USA; J. Brent Hiskey, University of Arizona, Col. of Eng. & Mines, PO Box 210072, Tucson, AZ 85721 USA

8:30 AM Keynote

Challenging the Traditional Hydrometallurgy Curriculum– An Industry Perspective: *Michael B. Mooiman*¹; David J. Kinneberg¹; Kathryn C. Sole¹; ¹Metalor USA Refining Corporation, 255 John Dietsch Blvd., PO Box 255, North Attleborough, MA 02760 USA

The hydrometallurgist's role in industry has changed considerably over the past 20 years. Flowsheet development is now a smaller component of the job and, more often than not, issues of operations management, environmental regulations, worker safety, risk assessment and finances are more important. Moreover, the narrowness of the curriculum defined by the term "hydrometallurgy" does not encompass the application of hydrometallurgical concepts to related fields such as surface finishing, recycling and the production of advanced materials by aqueous processing techniques. From an industry perspective, the traditional hydrometallurgy curriculum has shortcomings in preparing hydrometallurgists for an industrial career and changes are necessary.

9:05 AM Invited

Bringing Hydrometallurgy into a Global E-Learning Environment: J. Brent Hiskey¹; ¹University of Arizona, Col. of Eng. & Mines, PO Box 210072, Tucson, AZ 85721 USA

Hydrometallurgy, as a method of processing minerals and metals, dates back into antiquity. There are many early references of the application of solutions to ores and the treatment of mine waters. Surprisingly, hydrometallurgy as a branch of the academy is relatively recent. Certainly, elements of hydrometallurgy were presented as university subjects since the mid to late 1900th century. Only after the Manhattan Project (i.e. early 1950s) was curricula formally developed. During this period there is evidence of a strong underpinning in thermodynamics, kinetics, solution chemistry and equilibria, and engineering design. In recent years there has been emphasis on advanced techniques in simulation and modeling, computation fluid dynamics, application of advanced instrumentation, and integration of the biological sciences. Traditionally, hydrometallurgical education/training has been offered at small programs comprising one or two key faculty, and at highly distributed locations (Salt Lake City, Perth, Vancouver, Reno, Johannesburg). Furthermore clients for this discipline are equally small and distributed. With advances in high speed computing, refinements in graphic design tools, and expansion of the internet, distance education has taken on a new meaning in recent years and can hopefully reshape the way we teach hydrometallurgy. As a start two things need to be done in this arena, 1) sources must be linked together to develop meaningful curricula; and 2) clients and uses (both students and practitioners) must be connected with these sources. This paper highlights some of the special characteristics of the field of hydrometallurgy and suggests how the internet can bring about global collaborations. The TriUniversity Masters of Engineering program in Arizona represents one example of this type of collaboration and partnership. This program will be reviewed in the context of developing an elearning environment for hydrometallurgy.

9:30 AM Invited

Developments in the Teaching of Hydrometallurgy in Australia: *Michael J. Nicol*¹; ¹Murdoch University, Extractive Metall., South St., Murdoch, WAU 6050 Australia

The teaching of courses in geology, mining and extractive metallurgy in Australian universities is undergoing significant change largely as a result of the initiative taken by the Minerals Council of Australia(MCA). This has resulted in a major program aimed at developing national under- and postgraduate courses in selected areas with the aim of making these available to a consortium of participating universities. Murdoch university, together with the A J Parker CRC for Hydrometallurgy has been commissioned to develop the course in hydrometallurgy. Progress in the development of this course will be discussed in terms of overall philosophy, content and mode of delivery. Aspects of the extension to a Web-based course will also be summarized. Murdoch University has also established a hydrometallurgical pilot plant on the campus and the results of the first continuous operation for several months using under- and postgraduate students as operators will be discussed from the point of view of practical training and providing an interface with the local industry.

9:55 AM Invited

Teaching and Learning Aqueous Processing: A Brazilian Experience: Virginia S.T. Ciminelli¹; ¹Universidade Federal de Minas Gerais, Dept. of Metlgcl. & Matls. Eng., R. Espirito Santo, 35/s206, Belo Horizonte, MG Brazil

The evolution of Hydrometallurgical Education in Brazil is discussed in terms of the context and perspectives of the mining and metallurgical industries, the programs of interaction developed with industry, and research opportunities. Recent reorientation leading to a broader Aqueous Processing approach and a focus on environmental issues is also presented as well as strategies implemented to meet challenges in the competition for research funds and students.

10:20 AM Break

10:35 AM

Teaching Hydrometallurgy to Chemical Engineers and Chemical Engineering to Hydrometallurgists: *Matthew Ian Jeffrey*¹; ¹Monash University, Chem. Eng. Dept., Clayton, Victoria 3800 Australia

This presentation will discuss the teaching of Hydrometallurgy at Monash University in Victoria, Australia. Being based in a Chemical Engineering Department, the formal teaching of Hydrometallurgy to undergraduates is limited. A reasonable number of our graduates find work in the large Hydrometallurgy based industry in Australia, and hence it is important for them to learn about hydrometallurgical processes; our approach to this problem will be discussed. The presentation will also discuss some of the subjects which are taught to our Chemical Engineers, em phasing the importance of knowledge in subjects such as Process Control, Process Design and Reaction Engineering. It is the presenter's view that Hydrometallurgists should be trained in these areas. The teaching of research in Hydrometallurgy to both the undergraduate and postgraduate students will also be discussed.

11:00 AM Invited

Teaching Corrosion via the Internet using a Variety of Tools to Enhance Lear: Michael L. Free¹; ¹University of Utah, Dept. of Metlgcl. Eng., 135 S. 1460 E., Rm. 412, Salt Lake City, UT 84112 USA

An on-line corrosion course was designed and delivered with the goal of providing a high-quality learning environment for students. The course utilizes a variety of electronic and organizational tools such as a virtual laboratory, on-line quizzes, group projects, and multi-media lecture presentations to provide high quality educational opportunities for students. The course organization and development will be discussed and demonstrated.

11:25 AM Invited

The Virtual Laboratory: Reality or a Really Bad Idea: Saskia Duyvesteyn¹; R. Peter King¹; ¹University of Utah, Metlgcl. Eng., 135 S. 1460 E., Rm. 412, Salt Lake City, UT 84112-0114 USA

By simulating metallurgical equipment, processes and reactions, the Virtual Laboratory environment makes it possible for students to easily, quickly, conveniently and accurately perform laboratory experiments. Just as in a "real" lab, the student must select the necessary materials and appropriate operating parameters, then take readings/ samples during the experiment, and finally send the samples for analysis. Throughout these steps, the student must take decisions that impact the outcome of the results. Where the Virtual Lab outshines "reality" is that if a wrong decision is made, the experiment can be reset in a matter of seconds. In the last two years that the VLab has been utilized in our courses, we are noticing a substantial improvement in student performance. VLab also makes it possible to add a laboratory component to courses that traditionally have not been able to utilize labs because of time constraints or difficulty in undertaking the necessary experiments.

11:50 AM Closing Remarks