# TMS2004

**133rd Annual Meeting & Exhibition** 

The Minerals, Metals & Materials Society welcomes you to the TECHNICAL PROGRAM

for the 133<sup>rd</sup> TMS Annual Meeting & Exhibition, to be held March 14–18, 2004, in Charlotte, North Carolina.



For your convenience, we have also included details on

- Meeting Activities and Registration
- Conference Proceedings
- Our Exhibition
- **■** TMS Membership
- Additional On-line Resources that You May Utilize

All designed to help you prepare for— and optimally benefit from— one of the world's premier metals and materials events.

This document comprises

# THURSDAY'S TECHNICAL PROGRAM

Including fully text-searchable paper titles, abstracts, and author names with affiliations

**See you in Charlotte!** 





http://www.tms.org/ AnnualMeeting.html The Improved Web Resource for Every TMS Publication...

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  Gather individual papers and articles from TMS proceedings volumes, *JOM*, *Journal of Electronic Materials*, and *Metallurgical and Materials Transactions A* and *B* to create a one-of-a-kind publication that meets your needs. TMS will compile them in either a softcover book or on a CD-ROM—it's your choice.
- Coming in 2004: TMS Letters

  TMS Letters is a peer-reviewed, on-line-only journal featuring technical updates of hitherto unpublished research presented at TMS meetings. Available free-of-charge to TMS members (and by subscription to nonmembers), the journal comprises two-page technical updates, including text and graphics.

  Visit the TMS Document Center for additional information about TMS Letters!

See it for yourself!
Visit the new TMS Document Center today.

http://doc.tms.org

# AN INTERNATIONAL EVENT IN SCIENCE AND ENGINEERING

During the week of March 14-18, the 2004 TMS Annual Meeting & Exhibition will host approximately 4,000 science and engineering professionals, representing more than 70 different countries. They are convening at the Charlotte Convention Center to attend a field-spanning array of metals and materials symposia containing more than 200 sessions and 1,900 individual technical presentations.

# This year's meeting will feature programming by

- TMS Electronic, Magnetic & Photonic Materials Division
- TMS Extraction & Processing Division
- TMS Light Metals Division
- TMS Materials Processing & Manufacturing Division
- TMS Structural Materials Division
- TMS Education Committee
- TMS Young Leaders Committee
- ASM International's Materials Science Critical Technologies Sector
- International Titanium Association
- International Magnesium Association
- National Science Foundation
- TMS Public & Governmental Affairs Committee

In addition to the technical programming featured on the following pages, attendees will have the opportunity to

- **Tour** the Exhibition of more than 160 Companies Displaying New Products and Services
- Attend Special Lectures and Tutorials
- Participate in Short Courses on Metal Matrix Composites, Introduction to Nanomanufacturing and Nanotechnology, Technology Transfer Seminar, Smelter Grade Alumina from the Smelting Perspective and Computational Modelling for the Materials Professional
- **Enjoy** Special Luncheons, Dinners, and Social Functions, including events honoring Didier de Fontaine, R.J. Arsenault, A.L. Roytburd and Roger D. Doherty
- Network Extensively
- **Experience** the Charm and Amenities of Charlotte

Extensive details about these and all conference-related activities can be found on the 2004 TMS Annual Meeting Web Site.

# WANT TO BE PART OF THE ACTION?

# Registration is easy.

Just complete and mail or fax the Annual Meeting Registration Form that appears in this document. Or, visit the meeting web site to register immediately (and securely) on-line.

To register in advance, your submission must reach TMS not later than **February 16, 2004.** After this date, it will be necessary to register at the meeting site.

The **Westin Charlotte Hotel** is the TMS headquarters hotel. Special conference rates have been contracted with this hotel and others in the area surrounding the **Charlotte Convention Center.** To receive special rates, use the TMS 2004 Housing Reservation Form that appears in this document and that can be found on the meeting web site.

**Special Opportunity for TMS Nonmember Registrants:** All nonmember registrants automatically receive a one-year introductory associate membership in TMS for 2004. Membership benefits include a subscription to *JOM* (print and on-line versions) and significant discounts on TMS products and services.

More on the benefits of membership appears on the TMS Membership Web Pages.

# INTERESTED IN BUSINESS OPPORTUNITIES?

The 2004 TMS Annual Meeting & Exhibition presents businesses, universities, institutions, agencies, consultants, and others with myriad opportunities to partner in effective marketing communication. Such opportunities to reach thousands of meeting attendees include:

- Placing a **Booth** in the Exhibition
- Placing an Ad in the Official Conference Publication and At-Meeting Program: JOM
- Sponsoring High-Profile Attendee Services, such as the CyberCenter, Coffee Breaks, Signage, and Prize Drawings.
- Hosting a Hospitality Suite

More information on these opportunities is available on the 2004 TMS Annual Meeting Sponsorship Web Pages.

# **CONFERENCE** PROCEEDINGS: THE RECORDS OF EVENTS

The technical program of each TMS Annual Meeting yields numerous conference proceedings that document many presentations delivered in session rooms. Such publications can be ordered both before and after the meeting via the meeting registration form and/or the TMS Document Center.

The following symposium proceedings will be available in tandem with the meeting:

# ADVANCED MATERIALS FOR ENERGY CONVERSION II

Dhanesh Chandra, Renato G. Bautista, and Louis Schlapbach, editors ISBN 0-87339-574-3 • Approx. 560 pp., illus., index, softcover Order No. 04-5743 • Weight 3 lbs M \$112 + S \$89 + L \$160

# **ADVANCES IN SUPERPLASTICITY AND** SUPERPLASTIC FORMING

Eric M. Taleff, Paul E. Krajewski, and Peter A. Friedman, editors ISBN 0-87339-564-6 • Approx. 436 pp., illus., index, softcover Order No. 04-5646 • Weight 2 lbs M \$115 + S \$91 + L \$164

# **BULK METALLIC GLASSES**

Peter K. Liaw and Raymond A. Buchanan, editors ISBN 0-87339-573-5 • Approx. 256 pp., illus., index, softcover Order No. 04-5735 • Weight 2 lbs M \$125 + S \$99 + L \$179

# **EPD CONGRESS 2004**

Mark Schlesinger, editor

Includes the proceedings from the following symposia: Electrochemical Measurements and Processing of Materials, General Pyrometallurgy, Materials Processing Fundamentals, Solid and Aqueous Wastes, Sustainable Development session of Recent Advances in Non-Ferrous Metals Processing, and General Recycling session of Recycling.

ISBN 0-87339-565-4 • Approx. 1,020 pp., CD-ROM Order No. 04-5654-CD • Weight 1 lb M \$71 + S \$56 + L \$101

# **LATERITE NICKEL SYMPOSIUM 2004**

D.M. Lane and W.P. Imrie, editors ISBN 0-87339-550-6 • Approx. 1,144 pp., illus., index, hardcover Order No. 04-5506 • Weight 4 lbs M \$119 + S \$94 + L \$170

# **LIGHT METALS 2004**

A.T. Tabereaux, editor

Includes the proceedings from the following symposia Alumina & Bauxite, Aluminum Can Recycling, Aluminum Reduction Technology, Carbon Technology, Cast House Technology, Reactive Metals session of Recent Advances in Non-Ferrous Metals Processing, Aluminum and Aluminum Dross Processing

sessions of Recycling.
ISBN 0-87339-567-0 • Approx. 1,150 pp., illus., hardcover & CD-ROM
Order No. 04-5670-G • Weight 7 lbs M \$150 + S \$125 + L \$225

# **MAGNESIUM TECHNOLOGY 2004**

Alan A. Luo, editor

an A. Luc, editor.
ISBN 0-87339-568-9 • Approx. 436 pp., illus., hardcover & CD-ROM
Order No. 04-5689-G • Weight 3 lbs

M \$101 ★ \$ \$80 ★ L \$144

# SOLIDIFICATION OF ALUMINUM ALLOYS

Men G. Chu, Douglas A. Granger, and Qingyou Han, editors ISBN 0-87339-569-7 • Approx. 440 pp., illus., softcover Order No. 04-5697 • Weight 2 lbs M \$118 + S \$93 + L \$168

# **MULTIPHASE PHENOMENA AND CFD MODELING AND** SIMULATION IN MATERIALS PROCESSES

L. Nastac and B. Li. editors

Includes the proceedings from the following symposia: Multiphase Phenomena in Materials Processing and CFD Modeling and Simulation of Engineering

ISBN 0-87339-570-0 • Approx. 760 pp., illus., softcover Order No. 04-5700 • Weight 4 lbs M \$132 ← S \$105 ← L \$189

# SOLIDIFICATION PROCESSES AND MICROSTRUCTURES: A SYMPOSIUM IN HONOR OF PROF. W. KURZ

M. Rappaz, C. Beckermann, and R. Trivedi, editors ISBN 0-87339-572-7 • Approx. 432 pp., softcover Order No. 04-5727 • Weight 2 lbs M \$112 + S \$88 + L \$159

# THE FIFTH GLOBAL INNOVATIONS SYMPOSIUM ON MATERIALS PROCESSING AND MANUFACTURING: SURFACES AND INTERFACES IN NANOSTRUCTURED MATERIALS AND TRENDS IN LIGA, MINIATURIZATION, AND NANOSCALE MATERIALS

Sharmila M. Mukhopadhyay, John Smugeresky, Sudipta Seal, Narendra B. Dahotre, and Arvind Agarwal, editors

Includes the proceedings from the following symposia: Surfaces and Interfaces in Nanostructured Materials and the Fifth Global Innovations Symposium on Materials Processing and Manufacturing: Trends in LIGA, Miniaturization, and Nanoscale Materials

ISBN 0-87339-566-2 • Approx. 720 pp., illus., softcover Order No. 04-5662 • Weight 4 lbs M \$118 + S \$93 + L \$168

# **ULTRAFINE GRAINED MATERIALS III**

Yuntian Theodore Zhu, Terence G. Langdon, and Ruslan Z. Valiev, editors ISBN 0-87339-571-9 • Approx. 824 pp., illus., index, softcover Order No. 04-5719 • Weight 4 lbs M \$124 + S \$98 + L \$177

# M /Member + S / Student + L / List

# The following proceedings are planned for publication in TMS journals after the meeting:

# In the Journal of Electronic Materials

Challenges in Advanced Thin Films: Microstructures. Interfaces, and Reactions

Lead-Free Solders and Processing Issues Relevant to Microelectronic Packaging

Phase Stability, Phase Transformation, and Reactive Phase Formation in Electronic Materials III

# In Metallurgical and Materials Transactions

Beyond Nickel-Base Superalloys

Hume-Rothery Symposium: Structural and Diffusional Growth Phase Transformations and Deformation in Magnesium Alloys

# In TMS Letters

Processing and Properties of Powder-Based Materials

Other symposia eligible for TMS Letters:

Cost-Affordable Titanium

Dislocations

Educational Issues in Transport Phenomena in Materials Processing

General Abstracts

General Poster Session

Internal Stresses and Thermo-Mechanical Behavior in Multi-Component Materials Systems

Roytburd Symposium on Polydomain Stryctures

Symposium in Honor of Prof. Roger D. Doherty

The Didier de Fontaine Symposium on the Thermodynamics of Alloys

The Role of Grain Boundaries in Material Design

# ADDITIONAL RESOURCES

On-line answers to any of your 2003 TMS Annual Meeting & Exhibition questions can be found at

- 2003 TMS Annual Meeting & Exhibition Web Site: Get up-to-the-minute meeting details and complete registration materials at <a href="http://www.tms.org/AnnualMeeting.html">http://www.tms.org/AnnualMeeting.html</a>
- TMS Personal Conference Scheduler:

  Review the most-up-to-date version of the technical program, examine the calendar of events, and create your own personalized itinerary by visiting <a href="http://pcs.tms.org">http://pcs.tms.org</a>

vw.tms.org

- TMS Document Center: Review the complete tables of contents for conference proceedings and order publications by visiting <a href="http://doc.tms.org">http://doc.tms.org</a>
- **TMS Membership:** Learn more about the benefits of membership by touring <a href="http://www.tms.org/Society/membership.html">http://www.tms.org/Society/membership.html</a>
  - TMS Business-to-Business Partnering:
    Learn how TMS can help your organization
    maximize its impact by viewing
    <a href="http://www.tms.org/Meetings/Annual-04/Exhibit2004/Annual04-exhibit-home.html">http://www.tms.org/Meetings/Annual-04/Exhibit2004/Annual04-exhibit-home.html</a>

# If you want to contact a person, more details are available at

TMS Meetings Department
The Minerals, Metals & Materials Society
184 Thorn Hill Road, Warrendale, PA 15086 USA
Telephone: 1-800-759-4867 (in the U.S. and Canada) or
(724) 776-9000, ext. 243
Fax: (724) 776-3770

# TMSLETTERS



Timely, relevant, and rigorously reviewed, *TMS Letters* is a unique technical journal that presents cutting-edge research in succinct, informative technical updates.

The peer-reviewed journal will be available exclusively in on-line format through the TMS Document Center (*doc.tms.org*) and will be accessible free-of-charge to all TMS members as a benefit of membership. *TMS Letters* will be composed entirely of two-page technical updates, including text and graphics, of research presented at TMS meetings that are not published in any other book or journal.

The first issue of *TMS Letters* will consist exclusively of technical updates presented at the 2004 TMS Annual Meeting, to be held March 14–18, 2004. Presenters at the 2004 TMS Annual Meeting, whose work will not be published in any other book or journal, may submit their work for publication in the inaugural issue of *TMS Letters*.

To learn more about *TMS Letters* or to submit a technical update, contact:
Dan Thoma
Editor, *TMS Letters*c/o TMS
184 Thorn Hill Road, Warrendale, PA 15086
E-mail: tmsletters@tms.org

Web: www.tms.org/tmsletters.html

Visit this web site often, as more details will be made available throughout the year, including author instructions for submitting papers to the journal and non-member subscription information.

TMS2004	}
March 14-18 2004 • Charlotte N	$\mathbf{c}$

# ADVANCE REGISTRATION FORM Payment must accompany form.

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04-5646 Advances in Superplasticity a							\$115	\$164		
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# TMS2004

# 133rd Annual International Meeting & Exhibition March 14-18, 2004 • Charlotte, North Carolina, USA

Making your reservation is easier than ever through Travel Planners' real-time Internet reservation system! Just log on to www.tms.org, and follow the link to Travel Planners. You will be able to view actual

# **HOUSING RESERVATION FORM**

Mail or fax this housing form to:

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# Reservations must be received at Travel Planners by: Monday, February 16, 2004

Arrival Date		Departure Date		
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6 Marriott City Center Hotel \$138/Traditional S/D \$138/Concierge Level S/D	W. Trade St. E. Trade St. W. Fourth St. W. Third St. E. Third St. W. Second St. E. Second St. W. First St. E. First St.	CHARLOTTE CONVENTION CENTER East Stonewall St.	S. Caldwell N. Caldwell St. S. Davidson	Meeting & Exhibition by making your reservation at one of the listed hotels prior to the advance housing deadline. Thank you.  Confirmations: Confirmations will be e-mailed faxed or mailed to you from Travel Planners, Inconce your reservation has been secured with a deposit or credit card. You will not receive a confirmation from your hotel. If you do not receive a confirmation mithin 7 days, please call Trave Planners, Inc.  Changes/Cancellations: All changes and cancellations in hotel reservations must be made with Travel Planners, Inc. up until 3 business days prior to arrival and are subject to the individua hotel's cancellation policies. Cancellations and changes within 3 days of arrival MUST be made with your hotel directly. Many hotels are now imposing fees for early departure. This rate is set by each hotel and may vary accordingly Please reconfirm your departure date at the time of check-in.  Reservations/Deposits: All reservations are being coordinated by Travel Planners, Inc. Arrangements for housing must be made through Travel Planners, Inc. and NOT with the hote directly. Reservations via Internet, phone or fax will be accepted with a major credit card or deposit of one night's room and tax payable to Travel Planners, Inc. Chech must be drawn in US funds on a US bank. Nowire transfers will be accepted. Deposit policies are set by each hotel, and are outlined on your hotel confirmation.  Please read all hotel information prior to completing and submitting this form to Travel Planners, Inc. Keep a copy of this form. Use one form per room required. Make additional copies
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# **THURSDAY**

# Advanced Materials for Energy Conversion II: Thermoelectrics, Superconductors, and Piezoelectric Materials

Sponsored by: Light Metals Division, LMD-Reactive Metals Committee

Program Organizers: Dhanesh Chandra, University of Nevada, Metallurgical & Materials Engineering, Reno, NV 89557 USA; Renato G. Bautista, University of Nevada, Department of Chemical and Metal Engineering, Reno, NV 89557-0136 USA; Louis Schlapbach, EMPA Swiss Federal, Laboratory for Materials Testing and Research, Duebendorf CH-8600 Switzerland

Thursday AM Room: 203A

March 18, 2004 Location: Charlotte Convention Center

Session Chairs: Jeff Snyder, Jet Propulsion Laboratory-California, Thermoelect. Matls. & Devices Team, Pasadena, CA 91109-8099 USA; James L. Gole, Georgia Institute of Technology, Sch. of Physics, Atlanta, GA 30332-0430 USA; Chandra S. Pande, Naval Research Laboratory, Matls. Sci. & Tech. Div., Washington, DC 20375-5343 USA

# 8:30 AM Keynote

Advances in Thermoelectric Materials Leading to Reliable, Clean Energy Solutions: G. Jeffrey Snyder<sup>1</sup>; <sup>1</sup>Caltech/JPL, Matls. Sci., MS 277, Pasadena, CA 91109 USA

Thermoelectric generators, by converting waste heat into electricity, could be an important solution to today's energy challenges, but their applicability has been limited by the relatively low efficiencies. Solid state thermoelectric cooling devices are rapidly becoming more important for specialty applications. Advances in thermoelectric materials, design and device micro-engineering are rapidly expanding the promise of thermoelectrics. From a phenomenological and microscopic understanding of the thermoelectric effects, improved materials for thermoelectric applications can be engineered, with the ideal material having the electronic structure of a crystalline semiconductor but phonon structure of an amorphous material. The improved thermoelectric properties of many new thermoelectric materials, such as skutterudites and zinc antimonide, can be understood using this principle. Up to 20% thermal to electric conversion efficiency can be achieved by segmenting different materials over a wide temperature range. For segmented devices the compatibility factor, recently derived from the intensive formulation of efficiency, must also be considered for materials selection. Improved cooling performance can be achieved by taking advantage of the time dependence of the Peltier cooling effect or miniaturizing the cooler with MEMS technology.

# 8:55 AM

Thermoelectric Properties of Several P- and N-Type Half-Heusler Compounds and Effects of Dopants: Yumi Hayashi<sup>1</sup>; Sung Wng Kim<sup>1</sup>; Yoshisato Kimura<sup>1</sup>; Yoshinao Mishima<sup>1</sup>; <sup>1</sup>Tokyo Institute of Technology, Matls. Sci. & Engrg., 4259 Nagatsuta, Midori-ku, Yokohama-shi, Kanagawa-ken 226-8502 Japan

Half-Heusler compounds are attractive Phonon-Glass-Electron-Crystal thermoelectric materials applicable at high temperatures. They exhibit semiconducting properties at Valence Electron Count (VEC) of nearly 18. In the present work, we categorized all the available Half-Heusler compounds by VEC and selected several candidates by preliminary experiments. For instance, n-type HfNiSn and p-type TiFeSb are interesting because of their low thermal conductivity. Additionally, HfNiSn shows excellent seebeck coefficient. Twofold concept of our material design to effectively improve the thermoelectric figure of merit is; to reduce lattice thermal conductivity by alloying heavier elements substituting constitutional elements and to enhance the power factor by doping impurities. We previously reported successful alloy design of TiNiSn by alloying Hf and doping Sb. Sample preparation was conducted using powder metallurgy in order to further reduce thermal conductivity. Thermoelectric properties were evaluated by measuring seebeck coefficient, electrical resistivity and thermal conductivity at temperatures ranging from 300 to 1000 K.

# 9:15 AM

Thermoelectric Properties and Microstructure of p-Type Bi2Te3-Sb2Te3 Prepared by Powder Consolidation Using Equal Chan-

**nel Angular Extrusion**: *Jae-Taek Im*<sup>1</sup>; K. T. Hartwig<sup>1</sup>; Jeff Sharp<sup>2</sup>; <sup>1</sup>Texas A&M University, Mechl. Engrg., College Sta., TX 77840 USA; <sup>2</sup>Marlow Industries, Inc., 10451 Vista Park Rd., Dallas, TX 75238-1645 USA

Multipass Equal Channel Angular Extrusion (ECAE) was used to consolidate p-type Bi2Te3-Sb2Te3 powder prepared by milling cast material. The sieved powder was vacuum encapsulated and extruded in the temperature range of  $450\sim500^{\circ}\text{C}$ . The microstructure is characterized by polarized optical microscopy and SEM. The Seebeck coefficient, electrical resistivity, thermal conductivity, and the figure of merit were measured as a function of extrusion temperature and number of extrusion passes. The results are compared with thermoelectric properties and microstructure of cast and extruded material.

# 9:35 AM

The Enhancement of High Temperature Thermoelectric Properties of TiNiSn Based Half-Heusler Compounds: Sung Wng Kim<sup>1</sup>; Yoshisato Kimura<sup>1</sup>; Yoshinao Mishima<sup>1</sup>; <sup>1</sup>Tokyo Institute of Technology, Interdisplinary Grad. Sch. of Sci. & Engrg., Dept. Matls. Sci. & Engrg., 4259 Nagatsuta Midori-ku, Yokohama, Kanagawa 226-8502 Japan

In order to develop good thermoelectric materials for high temperature thermoelectric applications, a systematic investigation has been conducted on the high temperature thermoelectric properties of TiNiSn based half-Heusler compounds. This study is focused on the optimizing the high temperature thermoelectric properties, especially, reducing the lattice thermal conductivity by fabrication of solid solution and using powder metallurgy techniques. Also, effort to enhance power factor is performed by adding several dopants on TiNiSn-based half-Heusler thermoelectric material. Owing to the reduced lattice thermal conductivity by Hf alloying and to increased power factor by Sb doping, Ti<sub>0.95</sub>Hf<sub>0.05</sub>NiSn<sub>0.99</sub>Sb<sub>0.01</sub> compound prepared by using powder metallurgy technique showed ZT=0.78 at 770K, the highest dimensionless figure of merit for half-Heusler compounds reported so far.

# 9:55 AM Break

# 10:10 AM Invited

Recent Developments in Superconducting Materials for Energy Conversion: Khershed P. Cooper<sup>1</sup>; Harry N. Jones<sup>1</sup>; Chandra S. Pande<sup>1</sup>; <sup>1</sup>Naval Research Laboratory, Matls. Sci. & Tech. Div., Code 6325, 4555 Overlook Ave. SW, Washington, DC 20375-5343 USA

Superconducting materials are very important for the Energy industry. The promise of superconductors is the transmission of power with no or little loss. Significant progress has been made in the development of high temperature superconductors suitable for use at liquid nitrogen temperature. However, flux pinning problems remain and need better understanding and development of techniques to minimize the adverse effects. A relatively new superconductor, MgB2, was discovered recently. While not a high temperature superconductor, it has many attractive properties such as the absence of a "weak link" effect at the grain boundaries and can operate at liquid hydrogen temperature. However, the synthesis of MgB2 is not trivial and several routes to its fabrication into wire form are being pursued and will be discussed. Many technical problems in the development of these two classes of superconductors remain. The challenges and opportunities in the use of these materials will also be discussed.

# 10:30 AM

**Piezoelectric Thin Films for Energy Conversion in MEMS**: *D. F. Bahr*<sup>1</sup>; C. D. Richards<sup>1</sup>; R. F. Richards<sup>1</sup>; J. V. Martinez<sup>1</sup>; T. M. Sullivan<sup>1</sup>; <sup>1</sup>Washington State University, Mech. & Matls. Engrg., PO Box 642920, Pullman, WA 99164-2920 USA

Microscale power systems based on MEMS technology offer the possibility to deliver high power densities using batch manufacturing methods. MEMS are particularly attractive for developing structures which flex and bend as opposed to rotate and slide, and piezoelectric materials based on the titanate structure are a good example of how flexing thin film structures can convert mechanical to electrical energy in a small volume package. This presentation will describe the fabrication of thin film based piezoelectrics (such as PZT and a variety of doped derivative compounds) in MEMS and their application in the P3 power system, which utilizes an external combustion engine to covert thermal to mechanical to electrical work. The paper will focus on the control materials properties and their effects on the power production in a prototype device. A path to the optimization of the performance as a function of chemistry, structure, and orientation will be demonstrated.

# 10:50 AM

Thermal Energy Storage Investigations in Binary System of Neopentylglycol and Tris(Hydroxymethyl)Aminomethane: Wen-Ming Chien<sup>1</sup>; Dhanesh Chandra<sup>1</sup>; John Hansen<sup>1</sup>; <sup>1</sup>University of Nevada, Metallurgl. & Matls. Engrg., MS 388, Reno, NV 89557 USA

The organic crystalline materials, such as neopentylglycol (NPG) and tris(hydroxymethyl)aminomethane (TRIS), undergo solid-solid phase transitions and store the thermal energy have great potential for the passive solar building application. In this study, the phase diagram of Tris-NPG was constructed using Guinier X-ray diffraction and differential scanning calorimetry (DSC) data. It was found that below ~316 K, there is virtually no solubility of Tris in NPG or visaversa. Between ~316 K to 378 K a wide two-phase region is observed. The maximum solubility of NPG in Tris is 21%NPG at 398 K and that of Tris in NPG is 45% Tris at 413 K. The phase diagram exhibits a peritectic transformation at 423 K and eutectoid transformation at 400 K. The heat capacity measurement of the TRIS-AMPL solid solutions are also performed by using the DSC methods. Thermodynamic and crystal structure of solid solutions and components useful for thermal energy storage will be discussed.

# 11:10 AM

An Overview of Piezoelectric Composites: Michael Arthur Coleman<sup>1</sup>; Renato G. Bautista<sup>1</sup>; <sup>1</sup>University of Nevada, Metallurgl. Engrg., 1664 N. Virginia, MS 388, Reno, NV 89557 USA

Current technological trends have demanded new piezoelectric materials with increased performance capabilities. In order to satisfy these requirements, composite materials consisting of a piezoelectric component and another material have been produced. The secondary phases have been as varied as the potential applications from polymers to metals, glass, and other ceramics. These composite materials have been used to sense and create vibrations, change optical properties for fiber optic applications, activate displacement responses, and sense accelerations. As the uses for piezoelectric composites continue to expand so does the information available on their production and properties. To aid in understanding current trends, this review gives a description of some of the research currently underway in composite design and application.

# Advanced Materials for Energy Conversion II: Metal Hydrides V, Thermal Energy Storage and Containment Materials

Sponsored by: Light Metals Division, LMD-Reactive Metals Committee

Program Organizers: Dhanesh Chandra, University of Nevada, Metallurgical & Materials Engineering, Reno, NV 89557 USA; Renato G. Bautista, University of Nevada, Department of Chemical and Metal Engineering, Reno, NV 89557-0136 USA; Louis Schlapbach, EMPA Swiss Federal, Laboratory for Materials Testing and Research, Duebendorf CH-8600 Switzerland

Thursday AM Room: 204

March 18, 2004 Location: Charlotte Convention Center

Session Chairs: Stephen N. Paglieri, Los Alamos National Laboratory, Tritium Sci. & Engrg., Los Alamos, NM 87554 USA; Hiroyuki T. Takeshita, Kansai University, Fac. of Engrg., Suita, Osaka 564-8680 Japan; Eric H. Majzoub, Sandia National Laboratories, Analytical Matls. Sci. Dept., Livermore, CA 94550 USA

# 8:30 AM

Methane Cracking Properties of Nitrided Zr-Mn-Fe-Al Getters: Stephen N. Paglieri<sup>1</sup>; Joseph R. Wermer<sup>1</sup>; Erica J. Larson<sup>1</sup>; Hain Oona<sup>1</sup>; John D. Baker<sup>2</sup>; Aleta Hagman<sup>3</sup>; <sup>1</sup>Los Alamos National Laboratory, Tritium Sci. & Engrg., PO Box 1663, MS-C348, Los Alamos, NM 87544 USA; <sup>2</sup>Idaho National Environmental and Engineering Laboratory, ID USA; <sup>3</sup>Northwestern University, Evanston, IL 60208 USA

Methane was decomposed over 5 and 50 g beds of porous Zr-Mn-Fe-Al pellets (SAES St909), retaining carbon on the getter and releasing hydrogen. Steady state methane cracking efficiency varied between 20 and 100% depending on pretreatment conditions, carrier gas (nitrogen or helium), temperature (650-800°C), residence time, and methane concentration (0.25 or 5%). Cracking efficiency declined upon exposure to nitrogen, and increased at higher temperatures and longer residence time. XPS was employed to examine getter utilization and composition while XRD was used to relate performance to structural changes.

# 8:50 AM

Phase Stability and Structure of Zr-Fe SAES St198 Alloy in Hydrogen: Michael Arthur Coleman<sup>1</sup>; Dhanesh Chandra<sup>1</sup>; <sup>1</sup>University of Nevada, Metallurgl. Engrg., 1664 N. Virginia, MS 388, Reno, NV 89557 USA

The Phase stability of the SAES Getter St198, nominally  $Zr_2Fe$ , at elevated temperatures in a hydrogen environment is observed. In addition the susceptibility of  $Zr_2Fe$  and  $Zr_3Fe$  hydrides to disproportionation into  $Zr_2H_x$  for a range of temperatures is examined. Inelasti Neutron Scattering is used to identify  $Zr_2Fe$  and  $Zr_3Fe$  hydrides and deuterides.

# 9:10 AM

Heat Capacities and Phase Equilibrium of Pentaglycerine and Neopentylglycol Binary System: Wen-Ming Chien<sup>1</sup>; Argenta Price<sup>2</sup>; Dhanesh Chandra<sup>1</sup>; <sup>1</sup>University of Nevada, Metallurgl. & Matls. Engrg., MS 388, Reno, NV 89557 USA; <sup>2</sup>Yale University, New Haven, CT 06520 USA

Polyalcohols, such as pentaglycerine (PG) and neopentylglycol (NPG), are the thermal energy storage materials which reversibly absorb large amounts of heat during solid-state phase transitions and have the potential applications for solar buildings. In this study, the thermal properties of the solid-solid state phase transition for the pentaglycerine and neopentylglycol binary system have been investigated by using differential scanning calorimetry (DSC). The PG-NPG solid solutions have been cycled 5 times between -20°C to 100°C and the different scan rates at  $2^{\circ}\text{C/min},\,5^{\circ}\text{C/min}$  and  $10^{\circ}\text{C/min}$  have been performed. The onset temperatures decease as the %PG composition increases from 10%PG to 25%PG. In the 25%PG to 60%PG composition range, the onset temperatures increase as the %PG compositions increase. The lowest onset temperature occurs at 25%PG-75%NPG solid solution of 8.7°C at 10°C/min rate and 11.7°C at 2°C/min rate. The eutectoid occurs at 20.22°C of 40%PG-60%NPG solid solution. The heat capacity measurement of the PG-NPG solid solutions has also been performed by using the DSC method. The detail phase transitions and heat capacity equations will be presented.

# 9:30 AM Break

# 9:45 AM Cancelled

Application of Austenitic Stainless Steels to Hydrogen and Tritium Storage

# 10:05 AM Cancelled

Thermal Cycling and Creep Studies of AM50+Nd Magnesium Alloy Based Carbon Fiber, SiC Particulate and In-Situ Mg2Si Reinforced Hybrid Composites

# 10:25 AM

Energy Benefits of Using Nickel Aluminide Intermetallic Alloy Furnace Rolls and New Damper Controls at ISG Burns Harbor Plate's Annealing Furnace: Peter Angelini¹; Vinod Sikka¹; Mike Santella¹; Anthony Martocci²; John Mengel²; Larry Fabina²; ¹Oak Ridge National Laboratories, Metals & Ceram. Div., 1 Bethal Valley Rd., PO Box 2008, MS 6065, Oak Ridge, TN 37831 USA; ²ISG Burns Harbor Plate Inc. USA

At ISG Burns Harbor Plate Inc.'s, (formerly Bethlehem Steel Burns Harbor Plate Division) annealing furnace, new nickel aluminide intermetallic alloy rolls provide greater high-temperature strength and wear resistance compared to the conventional H series cast austenitic alloys currently used in the industry. This provides energy reduction based on slower roll speeds which allow greater hearth coverage and throughput, longer operating campaigns with fewer furnace light-ups, and improved surface finish of product which allows surface critical product to be processed at this furnace. Two commercial suppliers that followed rigid specifications produced the new alloy rolls. The team of Oak Ridge National Laboratory and ISG personnel developed these specifications. The nickel aluminide rolls are competitively priced with conventional H series alloy rolls. Twenty-nine new automated furnace control dampers have also been installed replacing older design, less effective pressure control dampers. These dampers, along with flame-safety control equipment and new AC motors and control equipment for improved roll speed control, are providing improved furnace control and additional energy efficiency.

# 10:45 AM Invited

Phase Equilibrium and Thermal Property Studies of Pentaerythritol and 2-Amino-2-Methyl-1,3-Propanediol Binary System: Wen-Ming Chien<sup>1</sup>; Dhanesh Chandra<sup>1</sup>; Renee Russell<sup>2</sup>; <sup>1</sup>University of Nevada, Metallurgl. & Matls. Engrg., MS 388, Reno, NV 89557 USA; <sup>2</sup>Pacific Northwest National Laboratory, PO Box 999, MS K6-24, Richland, WA 99352 USA

Thermal energy storage materials, "Plastic Crystals", reversibly absorb large amounts of heat during solid-state phase transitions. These

materials have potential applications in thermal energy storage for solar buildings. A binary phase diagram for Pentaerythritol (PE) and 2amino-2-methyl-1,3- propanediol (AMPL) is proposed. This diagram was determined by high temperature Guinier X-ray diffraction and differential scanning calorimetric (DSC) methods. The low temperature phases of PE and AMPL are in equilibrium between 293 K and 357 K in the composition range of 12 to 98 mol% AMPL. The phase diagram contains two eutectoids at 357 K and 420 K and a peritectic at 457 K. The solubility of AMFL in PE is very high, up to 45 mol% AMFL in PE at 420 K. The solubility of PE in AMFL is very low, only up to 10 mol% PE in AMFL at 357 K. The heat capacities of the PE-AMPL solid solutions are also obtained by using the DSC methods. The detail results obtained by X-ray diffractometry and DSC methods for the phase diagram and heat capacity data will be presented.

# **Aluminum Reduction Technology: Modeling**

Sponsored by: Light Metals Division, LMD-Aluminum Committee Program Organizers: Tom Alcorn, Noranda Aluminum Inc., New Madrid, MO 63869 USA; Jay Bruggeman, Alcoa Inc., Alcoa Center, PA 15069 USA; Alton T. Tabereaux, Alcoa Inc., Process Technology, Muscle Shoals, AL 35661 USA

Thursday AM Room: 213D

March 18, 2004 Location: Charlotte Convention Center

Session Chair: Vinko Potocnik, Vinko Potocnik Consultant,

Jonquiere, QC G7S 3C7 Canada

# 8:30 AM

An Improved Equation for the Interelectrode Voltage Drop in Industrial Aluminium Cells: J. Thonstad<sup>1</sup>; H.-D. Kleinschrodt<sup>2</sup>; H. Vogt2; 1Norwegian University of Science and Technology, Dept. of Matls. Tech., 7491 Trondheim Norway; 2TFH Berlin-University of Applied Sciences, D-13353, Berlin Germany

The interelectrode voltage drop is the largest single component making up the cell voltage in aluminium cells - except during anode effect. The presence of gas bubbles underneath the anode represents an increase in the ohmic resistance, and hence in the voltage drop across the electrolyte. It is common practice to estimate the interelectrode drop by taking into account the enhanced resistance in the gas bubble layer only, whereas the voltage drop in the essentially bubble-free region of the interelectrode space is treated as being unaffected by the presence of bubbles. An analysis shows that this procedure introduces a serious error. The large bubbles underneath the anode exhibit a strong effect on current distribution in the bubble-free region. Application of the finite-element method yields a practical relationship, demonstrating that the conventional procedure gives results for the interelectrode drop that are far too low.

# 8:55 AM

Numerical Modeling of Heat Exchanges Around an Aluminum Reduction Pot Shell: Thierry Tomasino<sup>1</sup>; Celine Martin<sup>1</sup>; Emmanuel Waz1; Steeve Renaudier1; 1Pechiney, Ctr. de Recherche de Voreppe, 725, rue Aristide Berges, BP 27, Voreppe Cedex 38341 France

The use of numerical modeling allows evaluation of working conditions and ventilation of electrolytic pots in the aluminum industry. But particular attention has to be paid to the correct analysis of all physical phenomena. A numerical 2D-model which integrates natural convection and radiation in order to describe the heat exchanges around an aluminum reduction pot shell, was developed with the commercial code FLUENT®. The temperature gradient between pot shell walls and ambient air generates a velocity field. The induced turbulent flow necessitates the use of a turbulence model associated to a wall function. The objectives of this work are to determine the best adapted models for both natural convection and radiation, and to consolidate results through different numerical tests. The numerical results are compared to correlations and measurements on pot. A good agreement is found.

Design Modification of Anode Super-Structure by Finite Element Analysis: M. M. Megahed<sup>1</sup>; H. S. Sayed<sup>1</sup>; F. M. Ahmed<sup>2</sup>; S. A. Mohamed2; A. Akhnokh2; 1Cairo University, Fac. of Engrg., Gamaa St., Giza Egypt; <sup>2</sup>Aluminium Company of Egypt, Nag-hammadi Egypt

The Aluminium Company of Egypt (Egyptalum) utilizes pre-baked anode cells with a current of 208 kA. Due to the relatively heavy weight of the existing anode steel structure, R&D at Egyptalum has recently conducted a detailed investigation with the objective of redesigning the anode superstructure to reduce its weight without sacrificing safety. Stress and deformation behaviors of the anode steel structure were investigated by means of finite element technique using shell elements. In addition to self-weight of the structure, weights of busbar, anode carbon, bunkers, lifting and jacking mechanisms, flexibles and crust effect were considered. Temperature variation was also taken into account. The results indicated that the existing anode structure posses a safety factor against yielding of about 7.5 and a safety factor against web buckling of at least 4.2. Thus an attempt was made to reduce anode weight via reducing flanges and web thickness of the anode section as well as the thickness of the trapezoidal gas passage section. Both static, thermal and buckling analysis were conducted by means of the FE model. The final design achieved a weight saving of about 14% with almost the same safety factors against static yielding or web buckling failure. This weight saving amounts to about 1200 kg of steel per anode.

# 9:45 AM

Two-Dimensional Model of Melt Flows and Interface Instability in Hall-Heroult Cells: Oleg Zikanov1; Haijun Sun1; Donald P. Ziegler<sup>2</sup>; <sup>1</sup>University of Michigan, Mech. Engrg., 4901 Evergreen Rd., Dearborn, MI 48128-1491 USA; <sup>2</sup>Alcoa, Primary Metals, Alcoa Techl. Ctr., 100 Techl. Dr., Alcoa Ctr., PA 15069-0001 USA

We derive a two-dimensional model for the melt flows and interface instability in aluminum reduction cells. The model is based on the de St. Venant shallow water equations and incorporates the essential features of the system such as the magnetohydrodynamic instability mechanism and nonlinear coupling between the flows and interfacial waves. The model is applied to verify a recently proposed theory that explains the instability through the interaction between perturbations of horizontal electric currents in the aluminum layer and the imposed vertical magnetic field. We investigate the role of other factors, in particular, background melt flows and magnetic field perturbations.

# 10:10 AM Break

# 10:20 AM

Demonstration Thermo-Electric and MHD Mathematical Models of a 500 kA Al Electrolysis Cell: Part 2: Marc Dupuis1; Valdis Bojarevics<sup>2</sup>; Janis Freibergs<sup>3</sup>; <sup>1</sup>GeniSim Inc., 3111 Alger St., Jonquiere, Quebec G7S 2M9 Canada; 2University of Greenwich, Sch. of Computing & Math., 30 Park Row, London SE10 9LS UK; 3University of Latvia, Inst. of Physics, 32 Miera St., Salaspils 2169 Latvia

In the present study, a full 3D cell thermo-electric model of a 500 kA demonstration cell has been developed and solved. In parallel, a non-linear wave MHD model for the full version of the same 500 kA demonstration cell taking into account the shielding effect of the detailed and optimized geometry of the potshell, is delivered. Preliminary results of the impact of the interactions between the cell thermoelectric and MHD models will be presented.

Magnetic Field in Electrolysis Cells and in the Potroom: Aureliu Panaitescu1; Augustin Moraru1; Ileana Panaitescu2; 1"Politehnica" University of Bucharest, Elect. Engrg. Dept., Splaiul Independentei 313, Bucharest 060032 Romania; <sup>2</sup>Isvor Fiat, Engrg. Processes & ICT, Corso Dante 103, Turin 10126 Italy

The knowledge of the magnetic field is important because its interaction with the current field in the molten media can induce instabilities; it can also affect the operation of electrical devices placed close to the pots. The mapping of the magnetic flux density values allowed the exposure level of the workers in the potroom to be assessed. The determination of stationary magnetic fields in nonhomogenous media with magnetic bodies is considered solved, but only for "local" methods. When the field is described in open domains the use of "integral" formulations is needed. In this area high performance methods of computation are still to be developed. One of them is described in this paper. The magnetic field obtained by our new code is compared with measurements performed inside the whole potroom. The comparisons showed good agreement. We obtained an engineering tool able to analyze the actual configuration and to be used also for the design of other electrolysis cells. The model created, both for complexity and accuracy of results, is a very good one among other known studies.

Busbar Optimization of High-Current Reduction Cells: Alexander Gusev1; Vassily Krioukovsky1; Leonid Krylov1; Vitaliy Platonov<sup>2</sup>; Petr Vabishchevich<sup>3</sup>; <sup>1</sup>RUSAL - Management Company, Mfg. Dept., 13/1 Nikoloyamskaya St., Moscow 109240 Russian Federation; 2Sayanogorsk Aluminium Smelter, Chakassia, Sajanogorsk 662793 Russian Federation; 3Russian Academy of Science, Inst. of Math. Modlg., 4 Miusskaya sq., Moscow 125047 Russian Federation

Busbar design optimization of high-current reduction cells is an important aspect of increasing the amperage. It is related to the fact that the actual busbar design does not provide satisfactory pot stability. For working out of different busbar optimization schemes Russian Aluminium uses a specially developed computer program Arc\@RusAl. Main feature of the program is accurate calculation of magnetohydrodynamic stability of pots on the basis of mathematic modeling of nonlinear dynamics of electrolyte-metal boundary. The involved mathematical models of the pot stability were verified on working pots by comparing calculated and measured pot stability reserve. On the basis of mathematic modeling we were able to work out several alternatives of busbar optimization. The recommended busbar modifications were implemented on a test group of pots. We obtained increased pot stability that, in turn, allowed achieving a significant reduction in pot voltage and metal level.

## 11:35 AM

Mathematical Modeling of Aluminum Reduction Cells in "Russian Aluminium" Company: G. V. Arkhipov<sup>1</sup>; <sup>1</sup>Russian Aluminum Company, Engrg. & Tech. Ctr. Russia

To give a comprehensive description of processing running in a cell an Ideal Mathematical Model is to solve interconnected problems of thermo-electric fields, magnetohydrodynamics, aerodynamics, strained-stress state, filtration of the melt and other problems. However, such a comprehensive model does not exist. There are models capable of calculating several fields interrelated with each other or in a certain sequence. The Engineering and Technology Center employs models to assess engineering solutions to retrofit and design cells with self-baking and prebaked anodes. Analysis of cells design involves the following modeling: thermo-electric field; strained-stress state; magnetic field; magnetohydrodynamics; aerodynamics of the air; electrical and heat balance.

# **Bulk Metallic Glasses: Mechanical Behavior**

Sponsored by: Structural Materials Division, ASM International: Materials Science Critical Technology Sector, SMD-Mechanical Behavior of Materials-(Jt. ASM-MSCTS)

Program Organizers: Peter K. Liaw, University of Tennessee, Department of Materials Science and Engineering, Knoxville, TN 37996-2200 USA; Raymond A. Buchanan, University of Tennessee, Department of Materials Science and Engineering, Knoxville, TN 37996-2200 USA

Thursday AM Room: 209A

March 18, 2004 Location: Charlotte Convention Center

Session Chairs: Jinn P. Chu, National Taiwan Ocean University, Matls. Engrg., Keelung, Taiwan 202 China; Christopher A. Schuh, Massachusetts Intitute of Technology, Matls. Sci. & Engrg., Cambridge, MA 02139 USA

# 8:30 AM Invited

Plastic Flow and Tensile Ductility of a Bulk Amorphous Zr55A110Cu30Ni5 Alloy in the Supercooled Liquid Region: Jinn P. Chu¹; Chun-Ling Chiang¹; Chang-Ting Lo¹; T. G. Nieh²; Y. Kawamura³; ¹National Taiwan Ocean University, Inst. of Matls. Engrg., 2 Pei-Ning Rd., Keelung 202 Taiwan; ²Lawrence Livermore National Laboratory, PO Box 808, Livermore, CA 94551 USA; ³Kumamoto University, Dept. of Mech. Engrg. & Matls. Sci., Kumamoto Japan

Tensile deformation behavior of a cast Zr<sub>ss</sub>Al<sub>10</sub>Cu<sub>30</sub>Ni<sub>5</sub> bulk metallic glass in the supercooled liquid region was investigated at strain rates ranging from 10<sup>-4</sup> to 10<sup>-2</sup> sec<sup>-1</sup>. The material exhibited excellent mechanical formability; a maximum tensile elongation of about 800% was recorded in the alloy at an initial strain rate of 10<sup>-2</sup>sec<sup>-1</sup>. The alloy was like a Newtonian behavior at high temperatures but to become non-Newtonian at low temperatures and high strain rates. The strain rate and temperature were found to play an important role in affecting deformation behavior of bulk Zr-based metallic glass in the supercooled liquid region. The strain rate sensitivity, i.e. the m value, was estimated to be ~0.9 under this test condition. Structures of the amorphous material, both before and after deformation, were examined using X-rays diffraction and high resolution transmission electron microscopy.

# 8:55 AM

Containerless Measurement of Thermophysical Properties of Ti-Zr-Ni Alloys: Robert W. Hyers<sup>1</sup>; Richard C. Bradshaw<sup>1</sup>; Jan R. Rogers<sup>2</sup>; Thomas J. Rathz<sup>3</sup>; Geun W. Lee<sup>4</sup>; Anup K. Gangopadhyay<sup>4</sup>;

Kenneth F. Kelton<sup>4</sup>; <sup>1</sup>University of Massachusetts, Dept. of Mech. & Industrial Engrg., 160 Governors Dr., Amherst, MA 01003 USA; <sup>2</sup>NASA Marshall Space Flight Center, Code SD46, Huntsville, AL 35812 USA; <sup>3</sup>University of Alabama, Huntsville, AL 35899 USA; <sup>4</sup>Washington University, Dept. of Physics, St. Louis, MO 63130 USA

The surface tension, viscosity, density, and thermal expansion of Ti-Zr-Ni alloys were measured for a number of compositions by electrostatic levitation methods. Containerless methods greatly reduce heterogeneous nucleation, increasing access to the undercooled liquid regime at finite cooling rates. The density and thermal expansion are measured optically, while the surface tension and viscosity are measured by the oscillating drop method. The measured alloys include compositions which form a metastable quasicrystal phase from the undercooled liquid, and alloys close to the composition of several multi-component bulk metallic glass-forming alloys. Measurements of surface tension show behavior typical of transition metals at high temperature, but a sudden decrease in the deeply undercooled liquid for alloys near the quasicrystal-forming composition range, but not for compositions which form the solid-solution phase first.

## 9:20 AM

Enhancement of Plasticity in Ni Based Bulk Metallic Glass Matrix Composites Containing Ductile Brass Phase: Minha Lee<sup>1</sup>; Dong Hyun Bae<sup>1</sup>; Won Tae Kim<sup>2</sup>; Do Hyang Kim<sup>1</sup>; Daniel J. Sordelet<sup>2</sup>; <sup>1</sup>Yonsei University, Metallurgl. Engrg., Ctr. for Noncrystalline Matls., 134 Shinchon-dong, Seodaemun-ku, Seoul 120749 Korea; <sup>2</sup>Chongju University, Physics, Chongju 360-764 Korea; <sup>3</sup>Iowa State University, Matls. Sci. & Engrg., Ames, IA 50014 USA

Centimeter scale Ni-based bulk metallic glass matrix composites were fabricated by warm extrusion of a mixture of gas-atomized fully amorphous powders and ductile brass powders. After consolidation, the composite retained the fully amorphous matrix found in the gas-atomized powder combined with the brass second phase. The confined ductile brass phase enabled the bulk metallic glass matrix composites to deform plastically under uniaxial compression at room temperature. However, control of the volume fraction and distribution of the ductile brass phase was important for the proper combination of the strength and plasticity. Formation of multiple shear bands during compressive straining was investigated to illustrate the enhanced ductility of the bulk metallic glass matrix composite containing ductile brass phase.

# 9:45 AM

**Deformation Behaviours of Bulk Amourphous Alloys During Hot Forming Processes:** *Yong-Shin Lee*<sup>1</sup>; S.-H. Yoon<sup>1</sup>; H.-G. Jeong<sup>2</sup>; <sup>1</sup>Kookmin University, Dept. of Mech. Engrg., 861-1 Chungneung-Dong, Sungbuk-Gu, Seoul 136-702 S. Korea; <sup>2</sup>KITECH, Dept. of Microforming S. Korea

Amorphous alloys are highly useful to realize high performance structural parts due to their excellent characteristics as functional and/ or structural materials, including the isotropic homogeneity free from crystalline anisotropy. Especially, their superior formability from the Newtonian viscous flow behaviour in the super cooled liquid state is very attractive in the view points of high precision forming. Such advantages of amorphous alloys have led researchers to work on manufacturing of highly precise, micro products like MEMS products. In this paper, thermo-mechanical finite element analyses are invoked to examine the deformation behaviours of Zr-based amorphous alloy and Pd-based amorphous alloy during hot forming processes such as hot forging and hot deep drawing. Comparisons of thermo mechanical deformation behaviours of amorphous alloys with those of superplastic materials will be also given.

# 10:10 AM

High Temperature Deformation and Hardening Associated to Partial Crystallization in Zr Based Bulk Metallic Glasses: Marc Bletry<sup>2</sup>; Qing Wang<sup>1</sup>; Jean-Jacques Blandin<sup>1</sup>; Pierre Guyot<sup>2</sup>; Yves Brechet<sup>2</sup>; Jean-Marc Pelletier<sup>3</sup>; Jean-Louis Soubeyroux<sup>4</sup>; <sup>1</sup>INP Grenoble, Génie Physique et Mécanique des Matériaux (GPM2), BP 46, Saint-Martin d'Hères 38402 France; <sup>2</sup>INP Grenoble, LTPCM, BP 75, Saint-Martin d'Hères 38402 France; <sup>3</sup>INSA de Lyon, GEMPPM; <sup>4</sup>CNRS Grenoble, CRETA

High temperature deformation of various Zr-based BMG were studied mainly in compression in the supercooled liquid region. The effects of temperature and strain rate were investigated, showing a transition from a Newtonian domain at low strain rate and/or high temperature to a non-Newtonian domain at high strain rate and/or low temperature. In the non-Newtonian domain, stress overshoots are generally obtained. The effect of composition on the deviations from the Newtonian behaviour is discussed and the mechanical behaviours of the BMG are interpreted thanks to a model taking into account the variation with experimental conditions of the free volume concentration.

Moreover, thermal treatments were also carried out to stimulate partial crystallization in the BMG and the behaviour of the resulting nano-composites was also investigated at high temperature. From such crystallization result important changes in the rheology of the BMG and these mechanical effects of partial crystallization are also discussed.

# 10:35 AM

Crystallization Behavior and Mechanical Properties of the Zr63Al7.5Cu17.5Ni10B2 Amorphous Alloy: Shian Ching Jason Jang<sup>1</sup>; <sup>1</sup>I-Shou University, Matls. Sci. & Engrg., 1, Sec. 1, Shiuecheng Rd., Dashu Shiang, Kaohsiung County, Taiwan 840 China

The crystallization behavior of Zr63Al7.5Cu17.5Ni10B2 amorphous Alloy was studied by means of scanning and isothermal differential calorimetry (DSC), X-ray diffraction (XRD), and transmission electron microscopy (TEM). A single stage transformation of the amorphous phase forming a Zr2Cu-type crystalline phase was observed. The activation energy for such a single stage crystallization of the amorphous phase was about 360±10 kJ/mole calculated by Kissinger analysis. Kinetics for the crystallization was analyzed by means of Johnson-Mehl-Avrami equation and discussed regarding to the value exponent obtained. The average value of Avrami exponent of 1.99 at the range from 694 to 700 K suggests that the nucleation mechanism is diffusion control with a decreasing nucleation rate. From the TEM analysis, small amount of Zr2Cu-type crystals in the nanoscale dimension (10-20 nm) were observed to precipitate from the amorphous matrix upon the early stage of isothermal heating the amorphous alloy at the temperature between the glass transition temperature and the crystallization. The fracture surface of bending the as-quenched amorphous ribbon 180° presents the typical ductile vein pattern. However, a ductile-brittle transition phenomenon occurs at the amorphous ribbon after 50% crystallization ratio of the isothermal annealing at the temperature between the glass transition temperature and the crystallization.

## 11:00 AM

Study of the Thermal Properties of Zr61Al7.5Cu17.5Ni10B4 Bulk Amorphous Alloy: Shian Ching Jason Jang<sup>1</sup>; L. J. Chang<sup>1</sup>; Y. T. Jiang<sup>1</sup>; T. F. Huang<sup>1</sup>; P. W. Wong<sup>1</sup>; <sup>1</sup>I-Shou University, Matls. Sci. & Engrg., 1, Sec. 1, Shiuecheng Rd., Dashu Shiang, Kaohsiung County, Taiwan 840 China

The ribbons of amorphous Zr61Al7.5Cu17.5Ni10B4 alloys with 0.1 mm thickness were prepared by melt spinning method. The thermal properties and microstructural development during the annealing of amorphous alloy have been investigated by a combination of differential thermal analysis, differential scanning calorimetry, high-temperature optical microscope, X-ray diffractometry and TEM. The glass transition temperature for the Zr61Al7.5Cu17.5Ni10B4 alloys are measured about 627 K (354?). This alloy also obtains a large temperature interval DTx about 86 K. Meanwhile, the calculated Trg for Zr61Al7.5Cu17.5Ni10B4 alloy presents the value of 0.57. The energy of crystallization for the activation Zr61Al7.5Cu17.5Ni10B4 was about 300 kJ/mol., as determined by the Kissinger and Avrami plot, respectively. The average value of the Avrami exponent n were calculated to be 1.99 0.45 for Zr61Al7.5Cu17.5Ni10B4 alloy.

# 11.25 AM

Research on Fracture Toughness of Fe-Based Bulk Amorphous Alloy: Huaxing Xiao<sup>1</sup>; Guang Chen<sup>2</sup>; <sup>1</sup>Changzhou Institute of Technology, No. 3, Changcheng Rd., Changzhou, Jiangsu 213002 China; <sup>2</sup>Nanjing University of Science and Technology, Jt. Lab. of Nanostructured Matls. & Tech., No. 200, Xiao-ling-wei, Nanjing, Jiangsu China

A plate bulk Fe-Co-Zr-Mo-W-B amorphous alloy with size of 20mm×10mm×1mm was prepared by arc melting mixtures of pure metals and metalloid B, inductive melting alloy ingots and using copper mold suction casting. The surfaces and fractures of the cast bulk amorphous alloy samples are of typical metallic luster. However, the obvious brittleness of the cast alloy makes it of little practical use. We use Vickers indentation technique to make a research on the amelioration of toughening on brittleness of the Fe-based bulk amorphous alloy. It is found that the fracture toughness of the alloy is raised from 1.6 MPa·m1/2 in the cast state to 4.5 MPa·m1/2 of the current situation. The mechanism of the toughness increase due to toughening in the BMG is discussed.

# Cast Shop Technology: Foundry

Sponsored by: Light Metals Division, LMD-Aluminum Committee Program Organizers: Corleen Chesonis, Alcoa Inc., Alcoa Technical Center, Alcoa Center, PA 15069 USA; Jean-Pierre Martin, Aluminum Technologies Centre, c/o Industrial Materials Institute, Boucherville, QC J4B 6Y4 Canada; Alton T. Tabereaux, Alcoa Inc., Process Technology, Muscle Shoals, AL 35661 USA

Thursday AM Room: 213B/C

March 18, 2004 Location: Charlotte Convention Center

Session Chair: Ian F. Bainbridge, University of Queensland, Co-op. Rsch. Ctr. for Cast Metals Mfg. (CAST), Brisbane, Qld 4072 Australia

# 8:30 AM

Monitoring of TiAlSi Particle Formation and Growth in Al-Si Alloys Using LiMCA: Martin Fortier<sup>1</sup>; X. Grant Chen<sup>1</sup>; <sup>1</sup>Alcan International Ltd., Arvida R&D Ctr., PO Box 1250, 1955 Blvd. Mellon, Jonquière, Québec G7S 4K8 Canada

The LiMCA (Liquid Metal Cleanliness Analyser) is a well-known equipment in the aluminum industry for the measurement of liquid metal cleanliness. It measures the size and number of particles less conductive than aluminum passing through a calibrated orifice. Titanium aluminides are intermetallic particles that are less conductive than aluminum. They commonly form and grow at high temperatures in Ti-contained aluminum alloys. A LiMCA was thus used inside a crucible of molten Al-Si foundry alloy in order to determine their formation temperature and growth kinetic. Results of the formation temperature are in good agreement with other methods. The growth kinetics of intermetallics is studied in detail in terms of the particle size change with both time and temperature. The use of the LiMCA was thus demonstrated as a tool for rapid evaluation of the formation and growth of intermetallic particles in liquid aluminum.

# 8:55 AM

Factors Influencing the Modification and Refinement of Hypereutectic Al-Si Alloys for Production of Automotive Pistons: Shahrooz Nafisi¹; Jalal Hedjazi²; S. M.A. Boutorabi²; Reza Ghomashchi¹; ¹University of Quebec, 555, Blvd. de l'Université, Chicoutimi, Québec G7H 2B1 Canada; ²Iran University of Science and Technology, Narmak, Tehran Iran

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

# :20 AM

Designing a High Quality Molten Aluminum System for the Production of High Volume Engine Block and Head Castings: Venky Srinivasan<sup>1</sup>; <sup>1</sup>GM Powertrain Division, Saginaw, MI USA

The push towards lightweight high performance engines in the automotive world has accelerated the conversion of iron blocks and heads to aluminum. As design engineers drive the requirement of high quality aluminum castings in automotive engines, foundry engineers in the automotive foundry industry are honing in their spotlight on melt quality. Quiescent metal transfer, metal level control, filtration degassing, redundancy during furnace re-lines and just in time liquid metal delivery are some of the key aspects to be considered while designing an integrated melt system for high quality automotive casting operations. This paper describes a systematic approach successfully used to design a cost effective high quality molten aluminum systems Lost Foam automotive block and head castings at GM Powertrain.

# 9:45 AM

Quality Piston Made from Hypereutectic Al-21% Si Alloy with Nodular Silicon Grains: Ru-Yao Wang<sup>1</sup>; Wei-Hua Lu<sup>1</sup>; Hsien-Yang Yeh<sup>2</sup>; Henry H.E. Yeh<sup>2</sup>; <sup>1</sup>Donghua University, Shanghai 200051 China; <sup>2</sup>California State University, Long Beach, CA 90840 USA

With excellent wear resistance and lower expansion, hypereutectic Al-Si alloy castings are suitable for car engine components, such as piston, cylinder line, engine block and others. As a general thumb, with silicon content wear resistance increases and expansion coefficient decreases. However, this alloy usually has coarse primary silicon with angular shape, which degrades mechanical properties and generates poor machinability, restricting its industry application. Now a procedure has been developed to modify the silicon in hypereutectic Al-Si alloys, in which the eutectic silicon appears with nodular shape and the primary silicon is rounded. The aim of this paper is to study the microstructural features of the piston made from the hypereutectic Al-22%Si alloy and the effect of nodular silicon grains on the mechanical and physical properties of the piston, its machinability and the bench test result.

# 10:10 AM

Directional Solidification of Aluminum Matrix Composites: Alicia Esther Ares²; Elvio de Napole Gregolin³; Rubens Caram⁴; Carlos Enrique Schvezov¹; ¹University of Misiones, Faculty of Sci., 1552 Azara St., Posadas, Misiones 3300 Argentina; ²CONICET, 1552 Azara St., Posadas, Misiones 3300 Argentina; ³Escola Politécnica da USP, Dept. de Engenharia Metalúrgica e de Materiais, Av. Prof. Mello Moraes 2463, Sao Paulo Brazil; ⁴State University of Campinas, Matls. Engrg. Dept., CP 6122, Campinas, Sao Paulo Brazil

It has been seen recently a progressive increase in the research of new techniques and processes for the obtention of metal matrix composites (MMC). This paper studies the directional solidification of Al-5SiO<sub>2</sub> fiber composite, due to its excellent mechanical properties and light weight. The columnar-to-equiaxed transition (CET) was observed in the samples directionally solidified from the chill zone in different solidification conditions. The transition occurs when the gradient in the liquid ahead of the columnar dendrites reaches values between -2.70°C/cm and -1.15°C/cm and the growth velocities reach values between 0.04 cm/s and 0.25 cm/s. The microstructure obtained is analyzed taking into account the characteristics of the alloy and the temperature profiles at the solidification interface. The followings tests were carried out on the composite: EDS, Vickers microhardness and optical microscopy. The results of the analysis are compared with those obtained in Al-Si binary alloys.

# Cost-Affordable Titanium Symposium Dedicated to Prof. Harvey Flower: Property Enhancement

Sponsored by: Structural Materials Division, SMD-Titanium Committee

Program Organizers: M. Ashraf Imam, Naval Research Laboratory, Washington, DC 20375-5000 USA; Derek J. Fray, University of Cambridge, Department of Materials Science and Metallurgy, Cambridge CB2 3Q2 UK; F. H. (Sam) Froes, University of Idaho, Institute of Materials and Advanced Processes, Moscow, ID 83844-3026 USA

Thursday AM Room: 206B

March 18, 2004 Location: Charlotte Convention Center

Session Chair: Vladimir A. Duz, ADMA Products Inc., Twinsburg, OH 44087 USA

# 8:30 AM

Applying Laser Powder Deposition for Reducing Costs in Titanium Fabrications: James William Sears<sup>1</sup>; <sup>1</sup>South Dakota School of Mines & Technology, Advd. Matls. Procg. Ctr., 501 E. St. Joseph St., Rapid City, SD 57701 USA

Laser Powder Deposition (LPD) is being evaluated for a variety of applications from aircraft sturctural components to medical implants. This paper will focus on recent work evaluating material response and process developments that are leading this technology towards qualification and acceptance as a manufacturing tool. The concept of using LPD as an Additive Manufacturing tool will be discussed. Basic enconmic models will also be presented.

# 9:00 AM

Ultra-High Pressure Warm Compaction for P/M Titanium Components: Hiroyuki Takamiya<sup>1</sup>; Mikio Kondoh<sup>1</sup>; Takashi Saito<sup>1</sup>; <sup>1</sup>Toyota

Central R&D Labs., Inc., Metallic Matls. Lab., 41-1 Yokomichi, Nagakute, Nagakute-cho, Aichi-gun, Aichi 480-1192 Japan

Blended elemental (BE) P/M process is one of an attractive method for obtaining cost affordable titanium components. However, the mechanical properties of the BE titanium products lose out to those of the wrought products mainly due to its residual pores. Furthermore, an excessive dimensional change (shrinkage) is inevitable to the sintering process, which spoils the dimensional precision and requires fatal cost increase in the final machining operation. For overcoming these shortcomings involved in the BE methods, we have developed a new process, ultra-high pressure warm compaction method. The key for the development is a discovery of metal die lubricant. Lithium Stearate shows a surprisingly super lubrication effect restricted at an elevated temperature of around 150°C with higher compacting pressure range from 600 MPa to 2,000 MPa. As a result, we could realize superior mechanical properties comparable to wrought products with an exact shaping (near zero shrinkage) in as sintered condition.

# 9:30 AM

Light Weight Powder Metallurgy Titanium-Magnesium-Aluminum Composites for Structural Applications: V. S. Moxson<sup>1</sup>; V. A. Duz<sup>1</sup>; J. S. Montgomery<sup>2</sup>; F. H. (Sam) Froes<sup>3</sup>; F. Sun<sup>3</sup>; <sup>1</sup>ADMA Products, Inc., 8180 Boyle Pkwy., Twinsburg, OH 44087 USA; <sup>3</sup>University of Idaho, Inst. for Matls. & Adv. Proc. (IMAP), McClure Hall, Rm. 437, Moscow, ID 83844-3026 USA

This paper describes new high performance and low density titanium alloy ADMATALTM-21 composites produced by innovative and low cost powder metallurgy approach using inexpensive titanium sponge fines, and 90%Mg-10%Al alloy. The ability to produce fully dense components with densities in the range of 2.7 gr/cm3-3.5 gr/cm3 has been demonstrated. Metallographic evaluation and chemical analysis of various phases was performed by scanning electron microscopy and electron probe analysis. Various microstructures of a 50%-75% skeleton of titanium and titanium alloys such as Ti-6Al-4V with a uniform distribution of 90%Mg-10%Al alloy will be presented. Eutectic Mg + Al12Mg17 phases with a lamela structure normally exist around the titanium and titanium alloy phase boundaries. These low density composite materials are potential candidates for automotive and aircraft applications as a substitution for aluminum and magnesium alloys.

# 10:00 AM Cancelled

Properties and Performances of Newly Developed High-Strength Alloy Series "Super-Tix TM"

# 10:30 AM

A Comparison of Titanium Powders from Various Sources: S. J. Gerdemann<sup>1</sup>; David E. Alman<sup>1</sup>; <sup>1</sup>Albany Research Center, Dept. of Energy, Albany, OR 97321 USA

The sintering behavior of titanium powder compacts made from gas atomized hydride-dehydride (HDH) and sponge powders were examined. Both CP and alloy titanium powders were considered. Compacts were vacuum sintered at 1200, 1275 and 1350°C for up to 960 minutes. The porosity and microstructure of the resulting sintered compacts were examined and the best conditions were used to produce tensile bars for mechanical testing. Some powders were also melted into buttons from which tensile bars were produced for comparison.

# 11:00 AM

Mechanism of Electrolytic Reduction of Titanium in Solid State in Molten Calcium Chloride Based Salts: S. Bliznyukov¹; R. Olivares¹; I. Ratchev¹; ¹BHP Billiton Minerals Technology, Newcastle, Off Vale S, Shortland, NSW 2307 Australia

Electrolytic reduction of titanium directly from solid TiO2 is a promising alternative to the current Kroll process. This new technology utilises an electrolytic cell, in which molten CaCl2-based salt is used as the electrolyte. A characteristic feature of this process is that the reduction of the feed material takes place in the solid state. Two version of the process have recently become popular, namely FFC and OS, advocated by Prof. D. Fray from Cambridge University and Prof. K. Ono and R. Suzuki from Kyoto University, respectively. The differently perceived mechanism of reduction ultimately may lead to significantly different cell designs and operating parameters. The present work is aimed at understanding the mechanism of titanium reduction as well as the limitations emanating from the process fundamentals.

# Failure of Structural Materials: General

Sponsored by: Structural Materials Division, SMD-Structural Materials Committee

Program Organizers: Michael E. Stevenson, Metals and Materials Engineering, Suwanee, GA 30024 USA; Mark L. Weaver, University of Alabama, Metallurgical and Materials Engineering, Tuscaloosa, AL 35487-0202 USA

Thursday AM Room: 211A

March 18, 2004 Location: Charlotte Convention Center

Session Chairs: Michael E. Stevenson, Metals & Materials Engineers, Suwanee, GA 30024 USA; Mark L. Weaver, University of Alabama, Metallurgl. & Matls. Engrg., Tuscaloosa, AL 35487-0202 USA

# 8:30 AM

Failure Analysis of Structural Metallic Bio-Implants: Michael E. Stevenson<sup>1</sup>; <sup>1</sup>Metals & Materials Engineers, 1039 Industrial Ct., Suwanee, GA 30024 USA

While the usage of advanced polymer compunds for use in structurcal orthopedic implants in increasing tremendously, metal alloys still comprise a substantial portion of the material used in structural biomaterials. This paper will discuss several failure analysis case studies of stainless steel and titanium alloy bio-implants. Topics of discussion will include alloy selection, mechanical design, installation, and usage.

# 8:50 AM

The Effect of Microstructure on Crack Initiation in Gamma-TiAl Sheet Materials: Shenavia Wilkerson Howell<sup>1</sup>; Viola L. Acoff<sup>1</sup>; University of Alabama, Metallurgl. & Matls. Engrg., PO Box 870202, Tuscaloosa, AL 35487 USA

Gamma TiAl sheet materials were investigated to characterize the initiation of cracks as a function of microstructure. The materials used in this study consisted of essentially the same composition, however, one was received in the primary annealed (PA) condition and the other in the designed fully lamellar (DFL) condition. All specimens were subjected to gas tungsten arc welding using a stationary torch (spot welding). For both conditions, all of the specimens cracked catastrophically immediately after welding, however, their mechanism of fracture was different. The fracture that occurred in the PA specimens followed an interdendritic path through regions that did not completely solidify prior to the occurrence of cracking whereas for the DFL specimens, the primary mechanism of fracture was cleavage. For both materials, a preferred growth of columnar grains was observed. The weld structure-property relationship will also be discussed.

# 9:10 AM

Failure Analysis of a Waste Burning Boiler Flue Gas Scrubber: Lindsey McCall<sup>1</sup>; Michael E. Stevenson<sup>1</sup>; <sup>1</sup>Metals & Materials Engineers, 1039 Industrial Ct., Suwanee, GA 30024 USA

The scrubber tower for a waste burning boiler at a power generation facility suffered a catastrophic failure subsequent to a series of intense storms. While failure had initially been attributed to the weather conditions alone, metallurgical failure anlaysis indicated that severe structural degradation due to corrosion was the root cause. This paper will discuss both the analysis of this failure and the general concepts of metallurgical failure analysis that prevent (or should prevent) arrival at erroneous inital findings pertaining to structural failure.

# 9:30 AM

A Thermal Ablation and Failure Model for Laser Cutting Operations: Ravindra Akarapu<sup>1</sup>; *Ben Li*<sup>1</sup>; Al Segal<sup>1</sup>; <sup>1</sup>Washington State University, Sch. of Mech. & Matls. Engrg., Pullman, WA 99164 USA

A mathematical model has been developed to perform the failure analysis of ceramic plates during dual laser cutting operations. The model development is based on the finite element simulations of thermal ablation and stress development during laser cutting. The integrated thermal and stress model is further integrated with the failure model to assess the thermal cracking during laser processing. The model development and numerical simulations are discussed and results are presented as a function of various laser cutting conditions.

# 9:50 AM Cancelled

Rheological Modeling of NanoIndentation and Verification of the Fracture Mechanics Principles for Multi-Layered Coatings

10:10 AM Break

# 10:40 AM

In-Situ Synchrotron X-Ray Microdiffraction Study of Dislocation Arrangements in Copper-Polycrystals During Uniaxial Deformations: Hyung-Don Joo¹; Chung-Wung Bark¹; Nobumichi Tamura²; Yang-Mo Koo¹; ¹Pohang University of Science & Technology, Ctr. for Advd. Aeros. Matls., Hyoja dong, Pohang, KyoungBook 790-784 S. Korea; ²Lawrence Berkeley National Laboratory, 1 Cyclotron Rd., MS 2-400, Berkeley, CA 94720 USA

The deformation of polycrystalline materials is very heterogeneous both at the intergranular and the intragranular level. Recent experiments have shown that formation of dislocation cell structure and rotation of structural elements at the marcro-level are fundamental to the development of plastic deformation and fracture of solids. However, in-situ study of deformation behavior in polycrystals at mesolevel has not been performed. In-situ measurement of local orientation and strain in Copper-polycrystals during uniaxial Deformations are investigated using synchrotron x-ray microdiffraction method at the Advanced Light Source of which beam size is 1.5micron \*1.5 micron. The intergranular heterogeneities of the deformation-induced microstructure were obtained. The shape of the intensity profile and the direction along elongated streaks in the Laue image are obtained at different positions of grain interior. The differences in the selection of simultaneously acting slip systems and that of dislocation arrangements among the intergranular and the intragranular level are discussed.

# 11:00 AM Cancelled

Computer Simulation of Rheological Modeling and its Application for Determining the Fracture of Multi-Layered Coatings

# 11:20 AN

Characterization of Plastic Deformation and Failure of Commercially Pure Titanium Via Disk Bend Testing: Patrick J. Henry<sup>1</sup>; Mark L. Weaver<sup>1</sup>; <sup>1</sup>University of Alabama, Metallurgl. & Matls. Engrg., Box 870202, Tuscaloosa, AL 35487-0202 USA

A disk bend test technique has been used to study deformation and failure mechanisms in commercially pure titanium. In the disk bend test, a 4 mm diameter X 0.5 mm thick disk is clamped around its rim in a circular holder and indented to failure with a flat aluminum oxide punch on its back face. The resulting behavior was compared with those from uniaxial compression and ball indentation tests. Differences and similarities in deformation between the disk bend and the compression tests are described.

# 11:40 AM

Fracture Toughness of Oxide Dispersion Strengthened Chromium Alloys: Mark L. Weaver<sup>1</sup>; Patrick J. Henry<sup>1</sup>; Joseph R. Hyde<sup>1</sup>; Jason K. Morgan<sup>1</sup>; <sup>1</sup>University of Alabama, Metallurgl. & Matls. Engrg., Box 870202, Tuscaloosa, AL 35487-0202 USA

This paper presents a study of the mechanical properties of sintered Cr-MgO alloys. The results show that limited room temperature ductility can be obtained in sintered commercial purity chromium by incorporating MgO particles. The results are discussed relative to the deformation of oxide dispersion strengthened metals and alloys.

# **General Abstracts: Session IX**

Sponsored by: TMS

Program Organizers: Adrian C. Deneys, Praxair, Inc., Tarrytown, NY 10591-6717 USA; John J. Chen, University of Auckland, Department of Chemical & Materials Engineering, Auckland 00160 New Zealand; Eric M. Taleff, University of Texas, Mechanical Engineering Department, Austin, TX 78712-1063 USA

Thursday AM Room: 201B

March 18, 2004 Location: Charlotte Convention Center

Session Chair: Eric M. Taleff, University of Texas, Mech. Engrg. Dept., Austin, TX 78712-1063 USA

# 8:30 AN

Comparison of Metallurgical and Acoustical Issues in Constructing and Tuning Stainless Steel and Brass Drums With a Caribbean Steel Drum Standard: L. E. Murr<sup>1</sup>; E. V. Esquivel<sup>1</sup>; A. C. Somasekharan<sup>1</sup>; C. A.C. Imbert<sup>2</sup>; R. Kerns<sup>3</sup>; S. Irvine<sup>3</sup>; S. Lowrie<sup>3</sup>; <sup>1</sup>University of Texas, Metallurgl. & Matls. Engrg., 500 W. Univ. Ave., El Paso, TX 79968 USA; <sup>2</sup>University of West Indies, Dept. of Mech. Engrg., Trinidad & Tobago, W. Indies; <sup>3</sup>Panyard, Inc., 1216 Calif. Ave., Akron, OH 44314 USA

Stainless steel (316L) and α-brass drums have been constructed along with a low-carbon (0.06% C) steel drum standard, by welding low-carbon steel sheet skirts (or cylindrical sides) and drum head sheet metal to 9 mm square carbon-steel hoops. The drum heads were all sunk to a depth of roughly 8.8 in. (22.3 cm) by pneumatic hammering to create a hemispherical-like note platform onto which a soprano drum pattern was developed and tuned. These drums are similar to the traditional Caribbean steel drum except the diameter is 23.5 in. (59.7 cm) instead of the standard 22.5 in. (57.2 cm) 55-gallon barrel. Microhardness profiles and drum head deformation features are compared along with optical metallographic and TEM observations of corresponding microstructures. Acoustical spectra for tuned notes common to each drum are examined. The results indicate that drums can be constructed and developed into musical instruments for a variety of metals, including hard aluminum alloys; especially where variations in the sound velocity are accommodated by appropriate alternations of note geometries as in the case of  $\alpha$ -brass.

# 8:55 AM

Correlation of Microstructure and Thermal Fatigue Properties of Centrifugally Cast High Speed Steel Rolls: Chang Kyu Kim¹; Jong Il Park²; Jae Hwa Ryu²; Jung Seung Yang³; Sunghak Lee¹; ¹Pohang University of Science and Technology, Ctr. for Advd. Aeros. Matls., San 31, Hyoja-dong, Namgu, Pohang, Kyungbuk 790-784 Korea; ²Pohang Iron and Steel Co., Ltd., Hot Rolling Dept., 1, Koedong-dong, Nam-gu, Pohang, Kyungbuk 790-600 Korea; ³INI Steel Company, R&D Dept., 444, Songnae-dong, Namgu, Pohang, Kyungbuk 790-707 Korea

In this study, thermal fatigue life of five different high speed steel rolls whose main composition had been modified were investigated by conducting the constraint thermal fatigue test. Five work roll materials which were manufactured by a centrifugal casting method were investigated quantitatively by microstructures, mechanical properties and thermal fatigue test. The basic microstructures of their shell regions were observed to be composed mainly of coarse primary carbides and tempered martensite matrix, and the cracks of thermal fatigue would initiate on primary carbides located on surface of the specimen and propagate along the primary carbides, and the thermal fatigue life of each roll was decreased with increasing the temperature range of the thermal fatigue cycles. These results were interpreted by the morphology of primary carbides and by cyclic softening phenomena associated with the exposed time at elevated temperatures during the thermal fatigue test.

# 9:20 AM

Morphology, Composition and Size Distribution of Inclusions in Fe-Si-Mn-Ti-Mg-Al-O-S Alloy Steels: Sang-Chae Park<sup>1</sup>; Chul-Ho Chang<sup>1</sup>; Han-Su Kim<sup>1</sup>; Hae-Geon Lee<sup>1</sup>; <sup>1</sup>Pohang University of Science and Technology, Dept. of Matls. Sci. & Engrg., San 31, Hyojadong, Nam-gu, Pohang, Kyungbuk 790-784 Korea

Morphology, composition, size and size distribution of inclusions/ precipitates formed during solidification and heats treating of Fe-Si-Mn-Ti-Mg-Al-O-S alloy steels were studied experimentally and the results were compared with thermodynamic prediction. Composition of the alloy, temperature and cooling rate were varied and the effects of these variables were determined quantitatively. For the Fe-Si-Mn-O-S system, inclusions/precipitates formed during solidification were mostly SiO<sub>2</sub>-MnO oxides having MnS phase in them. Depending on the cooling rate and isothermal holding time and temperature, a Mndepleted zone of the steel matrix was observed around these inclusions/ precipitates. These behaviors could be correctly explained through thermodynamic computation. If Ti was added, the proportion of SiO<sub>2</sub> in the oxide decreased and eventually disappeared to form MnO-TiO<sub>x</sub> compounds, When Ti content exceeded about 100ppm, only titanium oxide phases (Ti<sub>2</sub>O<sub>3</sub> or Ti<sub>3</sub>O<sub>5</sub>) formed. In existence of Ti, inclusions/ precipitates became smaller in size and were dispersed more evenly. In most cases, MnS phase were found attached to inclusions/precipitates. Addition of Mg(up to 52ppm) and Al(up to 148ppm) effected the change of composition and size of inclusions/precipitates to a large extent. Addition of Mg led to formation of MgO-TiOx and MgO oxides, depending on Mg content. Addition of Al modified oxides into MgO-Al<sub>2</sub>O<sub>3</sub> type of spinel. From the results of the present study the change of morphology, composition and size of inclusions/precipitates with steel composition and temperature were successfully mapped. Thermodynamic computation was found useful in predicting these changes and hence in designing steel compositions and thermal conditions for obtaining desired inclusions/precipitates.

# 9:45 AM

Thermally and Stress Induced Martensitic Transformation in New CoNiAl Shape Memory Alloys: H. Ersin Karaca<sup>1</sup>; Ibrahim Karaman<sup>1</sup>; Yuriy I. Chumlyakov<sup>2</sup>; <sup>1</sup>Texas A&M University, Dept. of

Mech. Engrg., MS 3123, College Sta., TX 77843 USA; <sup>2</sup>Siberian Physical-Technical Institute, Revolution Sq. 1, Tomsk 634050 Russia

In recent years ferromagnetic shape memory alloys have attracted increasing interest because of the ability to obtain one order of magnitude higher recoverable magnetic field induced strain (MFIS) than the other active materials. The main requirements for large magnetic field induced strain are: low twin boundary energy, high strength of matrix, high magnetocrystalline anisotropy energy and saturation magnetization. A recently discovered ferromagnetic shape memory CoNiAl alloy has promising shape memory characteristics for conventional and magnetic shape memory applications. In this study we have demonstrated that these alloys have low pseudoelastic stress hysteresis, high strength for dislocation slip, large pseudoelastic and two way shape memory strain, large pseudoelastic temperature window, and low stress for martensite reorientation. These findings satisfy the thermomechanical requirements to obtain MFIS. Additionally, high melting point, low density, good corrosion and oxidation resistance may result in the replacement of conventional SMAs with CoNiAl in most applications. This work is supported by Army Research Office, Contract No. DAAD 19-02-1-0261.

# 10:10 AM Break

# 10:20 AM

**Austenite Decomposition in Low-Carbon Fe-C-Mn Steels**: *R. E. Hackenberg*<sup>1</sup>; M. C. Gao<sup>2</sup>; D. G. Granada<sup>3</sup>; G. J. Shiflet<sup>2</sup>; <sup>1</sup>Los Alamos National Laboratory, Matls. Sci. & Tech. Div. (MST-6), MS G770, Los Alamos, NM 87545 USA; <sup>2</sup>University of Virginia, Dept. of Matls. Sci. & Engrg., 116 Engineer's Way, Charlottesville, VA 22904-4745 USA; <sup>3</sup>Nacional de Ingenieros Electromecanica, Tegucigalpa Honduras

Previous work on low-carbon Fe-C-Mn and Fe-C-Ni steels has documented kinetic, morphological and Mn partition-no partition transitions as a function of undercooling in the (first-to-appear) ferrite products. To better understand the correlations between these three transitions, the overall transformation kinetics, product morphologies and elemental distributions associated with the isothermal decomposition of austenite in Fe-(0.1, 0.2)C-(3, 4.2)Mn steels were surveyed using optical microscopy, SEM-EDS and TEM. Thermodynamic driving force calculations were done to better understand the undercooling at which these transitions took place. Additionally, the occurrence of carbide-rich products is documented, and similarities are drawn between select Fe-C-Mn steels that exhibit such carbide-rich products and betterknown steels that exhibit a bay on their TTT diagrams, such as Fe-C-Mo.

# 10:45 AM Cancelled

The Aging Behavior of a 24Cr-14Ni-2Mn Stainless Steel Under Nitrogen Atmosphere

# 11:10 AM

Heat Tinting of MADI(TM): Edward A. Druschitz<sup>1</sup>; Craig Johnson<sup>2</sup>; Alan P. Druschitz<sup>3</sup>; Heinrich Folz<sup>4</sup>; <sup>1</sup>Central Washington University, MET, 1042 Mistwood Place, Forest, VA 24551 USA; <sup>2</sup>Central Washington University, MET, 400 E. 8th Ave., Ellensburg, WA 98926 USA; <sup>3</sup>Intermet Corporation, 939 Airport Rd., Lynchburg, VA 24502 USA; <sup>4</sup>Intermet Neunkirchen Foundry, Postfach 14 18, Neunkirchen Germany

A metallographic technique has been developed to allow for the quantitative determination of the phases present in the microstructure of MADI(TM) (Machinable Austempered Ductile Iron). A correlation between the phases present and mechanical properties has also been determined. This technique and structure-property information are currently being used for production quality control and further material research and development.

# International Laterite Nickel Symposium - 2004: **Atmospheric Leaching**

Sponsored by: Extraction & Processing Division, EPD-Aqueous Processing Committee, EPD-Copper, Nickel, Cobalt Committee, EPD-Process Fundamentals Committee, EPD-Process Mineralogy Committee, EPD-Pyrometallurgy Committee, EPD-Waste Treatment & Minimization Committee

Program Organizer: William P. Imrie, Bechtel Corporation,

Mining and Metals, Englewood, CO 80111 USA

Room: 217B/C Thursday AM

March 18, 2004 Location: Charlotte Convention Center

Session Chairs: Vanessa de Macedo Torres, Companhia Vale do Rio Doce, Base Metals Projects Dept., Santa Luzia, MG 33030-970 Brazil; Roman M. Berezowsky, Dynatec Corporation, Ft. Saskatchewan, Alberta T8L 4K7 Canada

# 8:30 AM

Atmospheric Leaching of Laterites with Iron Precipitation as Goethite: Houyuan Liu1; Jim Gillaspie1; Coralie Lewis1; David A. Neudorf<sup>2</sup>; Steve Barnett<sup>3</sup>; <sup>1</sup>BHP Billiton, Newcastle Tech. Ctr., off Vale St., Shortland, New South Wales NSW 2307 Australia; <sup>2</sup>Hatch Canada, Hydrometall., 2800 Speakman Dr., Mississauga, ON L5K 2R7 Canada; <sup>3</sup>BHP Billiton, Queensland Nickel, 123 Eagle St., Brisbane, Queensland 4000 Australia

A new process was developed to recover nickel and cobalt by leaching laterite ore at atmospheric pressure and 95-105°C. The nickelcontaining goethite in limonite is firstly leached with sulphuric acid to liberate over 90% of nickel, cobalt and iron. The dissolved iron was then precipitated as Ni-free goethite with addition of saprolite. The acid released during iron precipitation is simultaneously used as lixiviant to leach saprolite to recover more nickel. With this process the limonite and saprolite are essentially converted into goethite-, gypsumand silica- containing tailings. Twenty bench tests and two campaigns of pilot plant operation (Capacity: 400 kg dry ore/day) were carried out at the BHP Billiton Newcastle Technology Centre (NTC) from January to August 2002. The overall nickel and cobalt extractions were 81-90% and 91-100% respectively. The average plant availability was 99%. The robustness of this process are most notably the very high plant availability, high consistency and simplicity of the operation.

A Fundamental Study of the Leaching of Pre-Reduced Laterites in Ammoniacal Solutions: Michael J. Nicol1; Aleksandar N. Nikoloski<sup>2</sup>; John E. Fittock<sup>3</sup>; <sup>1</sup>Murdoch University, Parker Ctr., South St., Murdoch, Western Australia 6050 Australia; <sup>2</sup>BHP Billiton, QNI Pty Ltd, PMB 5, Mail Ctr., Townsville, Queensland 4818 Australia; <sup>3</sup>BHP Billiton, QNI Pty Ltd, PMB 5, Mail Ctr., Townsville, Queensland

The recovery of nickel and cobalt by reduction roasting followed by leaching of the metallic iron-alloy grains in ammonia-ammonium carbonate solution remains as a robust, technically advanced process for the treatment of lateritic ores. The chemistry of the leaching of nickel and cobalt is linked closely with the dissolution and precipitation of the iron. Recently published results have shown that iron is prone to passivation in solutions typical of those used in practice and the passivation has been confirmed in actual leaching reactors. This passivation has been shown to be due to the formation of cobalt and nickel sulphide layers as a result of the reduction of thiosulfate present in the leach solutions. This paper will focus on other fundamental aspects of the leaching process such as the role of dissolved oxygen and cobalt(III) ions in the oxidation of the reduced alloy particles. In addition, options for minimizing the extent of passivation and optimising the rate of leaching have been investigated and will be discussed in the light of the fundamental findings.

# 9:20 AM

Direct Atmospheric Leaching of Saprolitic Nickel Laterite Ores with Sulphuric Acid: Walter Curlook<sup>1</sup>; <sup>1</sup>University of Toronto, Matls. Sci. & Engrg., 184 College St., Toronto, ON M5S 3E4 Canada

An atmospheric acid leaching process for leaching nickel and cobalt from highly-serpentinized saprolitic fractions of nickel laterite deposits has been developed and patented. The process involves leaching the highly-serpentinized saprolitic portion of the nickel laterite ore profile in strong sulphuric acid solutions at atmospheric pressure and temperatures between 80°C and 100°C, essentially autogenously, to extract over 85% of its contained nickel content and a large proportion of its cobalt content after leaching reaction times of about one hour. The amount of sulphuric acid used in the leaching process is between about 80% and 100% by weight of the finely ground highlyserpentinized saprolite ore on a dry weight basis. The metal values are recovered as intermediate products.

9:45 AM Break

# International Laterite Nickel Symposium - 2004: Slurry Rheology, Solution Extraction and Other

Sponsored by: Extraction & Processing Division, EPD-Aqueous Processing Committee, EPD-Copper, Nickel, Cobalt Committee, EPD-Process Fundamentals Committee, EPD-Process Mineralogy Committee, EPD-Pyrometallurgy Committee, EPD-Waste

Treatment & Minimization Committee

Program Organizer: William P. Imrie, Bechtel Corporation, Mining and Metals, Englewood, CO 80111 USA

Thursday AM Room: 217B/C

March 18, 2004 Location: Charlotte Convention Center

Session Chairs: Larry E. Seeley, President & CEO, SGS Lakefield Research Limited, Lakefield, Ontario K0L 2H0 Canada; Peter G. Mason, Falconbridge (Australia), Toowong, QLD 4066 Australia

A Study Utilising Vane Yield Rheometry to Predict Optimum Thickener Performance Across a Range of Laterite Nickel Ores for the Ravensthorpe Nickel Project: Lincoln Charles McCrabb1; Julian Chin<sup>1</sup>; Geoff Miller<sup>2</sup>; <sup>1</sup>Rheochem Ltd/BHP Billiton, 1 Keegan St., O'Connor, Western Australia 6163 Australia; <sup>2</sup>BHP Billiton, Level 200 St. Georges Terrace, Perth, Western Australia 6850 Australia

Correct measurement and interpretation of viscosity data is critical for design of any thickening and pumping process that involves a non Newtonian slurry. The nickel laterite pressure acid leach process relies on producing a slurry of maximum achievable solids concentration. Small variations of 1-2% solids concentration can alter economics significantly. For the Ravensthorpe Nickel Project, a rheology protocol has been developed which optimizes the solids concentration across a range of ore types. The vane yield stress technique has been utilized to accurately quantify the flow of thickened slurry in the lower shear range. A yield stress of 100Pa has been used as a benchmark to determine the optimum solids concentration achievable utilizing deep cone thickening. Statistical analysis of the data shows critical rheology distinctions between ore type, particle size, lithology and geochemistry. Linear and power law models have been applied to rheology flow curves to reconcile the material transport properties with the anticipated thickener underflow solids concentration.

Flow Array for Nickel Laterite Slurry: Donald J. Hallbom<sup>1</sup>; Bern Klein<sup>2</sup>; <sup>1</sup>Pipeline Systems Inc., 460 N. Wiget Ln., Walnut Creek, CA 94598-2408 USA; <sup>2</sup>University of British Columbia, Mining Engrg., 5th Floor, 6350 Stores Rd., Vancouver, BC V6t 1Z4 Canada

Limonitic nickel laterite forms time-dependent slurry with complex properties that vary from thixotropy to anti-thixotropy. Stress decay tests indicate that laterite slurry takes roughly two minutes to approach steady state after a step change. As a result, most rheometer measurements are taken at a non-equilibrium state. Two minutes is also long relative to the time that a unit of slurry is at any given shear rate in a processing plant, so the slurry may never reach equilibrium. Chronic problems may occur if designers and operators fail to take this into account. This paper presents the rheology of laterite slurry using a flow array, which describes the rheology using an array of instantaneous flow curves crossed by an equilibrium flow curve along with the structure change rates. This flow array allows the flow behavior of time-dependent slurry to be predicted in non-equilibrium conditions using a simple time-step methodology.

Manganese Separation by Solvent Extraction in Nickel Laterite Processing: Chu Yong Cheng1; Mark D. Urbani1; Martin Houchin1; <sup>1</sup>CSIRO, Div. of Minerals, PO Box 90, Bentley, Western Australia 6982 Australia

The separation of manganese from nickel and cobalt is reviewed and new solvent extraction processes for manganese separation are discussed. The use of intermediate precipitation, solids/liquid separation and re-leach in the three WA nickel laterite plants make these processes complicated and costly in capital and operation. By using a new synergistic organic system in semi-continuous tests with a pilot plant leach solution, Ni and Co together with zinc and copper were separated from the Mn, Mg, Ca and Cl) in the first SX circuit by extraction and scrubbing, indicating that manganese can be completely separated from nickel and cobalt using a synergistic solvent extraction approach. Semi-continuous test work with D2EHPA and synthetic and pilot plant leach solutions showed that manganese, together with calcium, copper and zinc can be effectively and efficiently separated from nickel, cobalt and magnesium by extraction, scrubbing and stripping.

#### 11:15 AM

Separation of Ni and Co from Ca, Mg and Mn in Sulphate Laterite Leach Solutions: Erin N. Legault-Seguin<sup>1</sup>; Akram M. Alfantazi<sup>2</sup>; Werner Dresler<sup>1</sup>; <sup>1</sup>Laurentian University, Sch. of Engrg., Ramsey Lake Rd., Sudbury, ON P3E 2C6 Canada; <sup>2</sup>University of British Columbia, Dept. of Metals & Matls. Engrg., Vancouver, BC V6T 174 Canada

The current industrial practice in the processing of nickeliferous laterites involves the precipitation and releaching of Ni and Co to allow separation from the major impurities of Mn, Mg and Ca. A direct solvent extraction process has significant advantages over this practice, which suffers from difficult and costly precipitation steps, lower recovery and inherently complex flowsheets. The present investigation involves the examination of Cyanex 272, Cyanex 301 and Cyanex 302 as extractants for the direct extraction of Ni and Co from major impurities associated with laterite leaching, i.e. Mn, Mg and Ca. For Co extraction, Cyanex 301 and Cyanex 302 are superior to Cyanex 272, because they are able to selectively separate Co from Mn, Mg and Ca. Cyanex 272 offers complete extraction of Co from Ni and Ca, but Mn and Mg pose difficulty. Ni can only be extracted selectively with Cyanex 301, thus another extractant selective for Ni, such as Versatic 10 or Cyanex 301, is needed to recover Ni if Cyanex 302 or Cyanex 272 is used for the initial extraction.

#### 11:35 AM

Solvent Extraction Technology for the Extraction of Nickel Using LIX 84-I. An Update and Circuit Comparisons: *J. Murdoch Mackenzie*<sup>2</sup>; Michael J. Virnig¹; ¹Cognis Corporation, Mining Chem. Tech., 2430 N. Huachuca Dr., Tucson, AZ 85745 USA; ²Cognis Australia, Mining Chem., 284 Victoria Rd., Malaga, Western Australia 6062 Australia

Two commercial nickel solvent extraction plants treating laterite leach solutions and using LIX® 84-I have been operated in Australia. These circuits employ similar extraction chemistry but differ in their leaching and stripping operations. An alternative process involving elements of both can also be conceived. The preparation of the feed solution to solvent extraction plays an important role in nickel extraction using LIX®84-I and the special features of manganese removal and cobalt oxidation in the preparation of the PLS is discussed. This paper compares these three circuit configurations with special reference to the extraction and reductive stripping of cobalt, the advantages and the transfer of zinc and copper to the strip aqueous, ammonia transfer, and sulfur transfer. In addition, the relative advantages and disadvantages of using a mixed hydroxide product as compared to roast reductive leaching approach or mixed sulfide precipitation approach will be considered. The potential degradation of the circuit organic is discussed along with measures to counter the effects of this degradation, such as Co stripping and re-oximation.

# Magnesium Technology 2004: Alloy Development

Sponsored by: Light Metals Division, LMD-Magnesium Committee Program Organizer: Alan A. Luo, General Motors, Materials and Processes Laboratory, Warren, MI 48090-9055 USA

Thursday AM Room: 203B

March 18, 2004 Location: Charlotte Convention Center

Session Chairs: Bob R. Powell, General Motors Corporation, Warren, MI 48090-9055 USA; Mihriban O. Pekguleryuz, McGill University, Montreal, QC H3A 2B2 Canada

# 8:30 AM

Magnesium Alloys for High Temperature Applications-An Overview: Mihriban O. Pekguleryuz¹; ¹McGill University, Metals & Matls. Engrg., 3610 Univ. St., Wong Bldg., Montreal, Quebec H3A 2B2 Canada

New growth area for automotive use of magnesium is powertrain applications such as the transmission case and engine block. These

applications see service conditions in the temperature range of 150-200C under 50-70 MPa of tensile and compressive loads. In addition, metallurgical stability, fatigue resistance, corrosion resistance and castability requirements need to be met. A decade of research and development has resulted in a number of creep-resistant magnesium alloys that are potential candidates for elevated-temperature automotive applications. These alloys are mostly based on rare-erath and alkaline earth elemnt additions to magnesium. This paper gives an overview of the various magnesium alloy systems for use in elevated-temperature applications.

#### 8:50 AM

The Influence of Sb, Si and Sn on the Mechanical Properties of Mg-Al Alloys: Per Bakke<sup>1</sup>; Ketil Pettersen<sup>2</sup>; Darryl Albright<sup>3</sup>; <sup>1</sup>Norsk Hydro, CC Magnesium, PO Box 2560, Porsgrunn N-3907 Norway; <sup>2</sup>Norsk Hydro, Corp. Rsch. Ctr., PO Box 2560, Porsgrunn N-3907 Norway; <sup>3</sup>Hydro Magnesium Marketing, 39209 W. Six Mile, Ste. 200, Livonia, MI 48152 USA

Magnesium die casting alloys based on Al as the main alloying element can broadly be grouped into two categories, depending on whether the third element(s) form stable phases with Al or Mg. Alloys with Ca (AX), Sr (AJ) and RE (AE) belongs to the first category, while alloys with Si (AS), Sn (AT) and Sb are examples from the second. This paper addresses alloying additions which form precipitates with magnesium, specifically within the Mg-Al-Sn-(Mn), Mg-Al-Si and Mg-Al-Si-Sb systems. The results show that for some Mg-Al-Sn(-Mn) alloys tensile yield- and ultimate tensile strength better than AZ91 can be obtained. The microstructure of the Mg-Al-Sn alloys consists of an a-Mg matrix with Al and Sn in solid solution, and a grain boundary eutectic of Mg-Mg2Sn. With increasing Al-content, the Mg2Sn phase is pushed into pockets at the grain nodes, and their effect on grain boundary pinning gradually vanishes. The creep resistance increases with increasing Sn or Sb-content, and alloys with creep properties better than AS21X can be obtained. However, with increasing contents of Al, this effect is significantly reduced.

#### 9:10 AM

Nucleation, Precipitation and Strengthening Mechanisms in Mg-Zn-Sn Based Alloys: Alexander Katsman<sup>1</sup>; Shalom Cohen<sup>1</sup>; Ginat R. Goren-Muginstein<sup>1</sup>; Menahem Bamberger<sup>1</sup>; <sup>1</sup>Technion, Matls. Engrg., Technion City, Haifa 32000 Israel

This work deals with the development of Mg-Zn-Sn based alloys with enhanced creep properties at elevated temperatures. This is achieved by precipitation of binary phases MgZn and Mg<sub>2</sub>Sn during the aging of these alloys. Mg-alloys with different amounts of Zn (0.8÷1.7 at.%) and Sn (0.7÷2at.%) were solution treated at 465°C for 96 hours and then water quenched. Aging at 175°C, 200°C, 225°C and 250°C up to 96 hours has led to the precipitation of the binary phases MgZn and Mg<sub>2</sub>Sn. The formation of these phases was studied experimentally (by XRD, SEM and hardness measurements). The Modified Langer-Schwartz approach, taking into account nucleation, growth and coarsening of the new phase precipitations, was used for analysis of the structural changes during aging. Simultaneous formation of the binary MgZn and the Mg<sub>2</sub>Sn phases was considered. Two maxima of hardness during the aging were found to be connected with the formation and coarsening of two types of precipitates. Densities, average size of precipitates and activation energies of the phase formation processes, which determine the strengthening mechanisms, were estimated. A reasonable agreement between the calculations and observations was found.

#### 9:30 AM

Phase Formation, Precipitation and Strengthening Mechanisms in Mg-Zn-Sn and Mg-Zn-Sn-Ca Alloys: Shalom Cohen<sup>1</sup>; Ginat R. Goren-Muginstein<sup>1</sup>; Shaul Avraham<sup>1</sup>; Menahem Bamberger<sup>1</sup>; <sup>1</sup>Technion, Matls. Engrg., Technion City, Haifa 32000 Israel

The trend towards weight reduction in transportation equipment has led vehicle manufacturers to produce various components made of Mg alloys. The need for light and strong components that can serve also under relatively elevated temperatures, has led an effort to develop new Mg base alloys. The requirements from the new alloys are a stable structure and good mechanical properties when exposed to elevated temperatures. Based on those demands a new family of Mg-Zn-Sn alloys is been developed. Studying the ternary and quaternary phase diagrams of the above system shows that Mg<sub>2</sub>Sn and several Mg-Zn intermetallics precipitate. An Mg-5%Sn-5%Zn alloy was chosen for a microstructure examination and precipitation hardening study. The addition of Ca to the basic Mg-Zn-Sn alloy was also studied based on the assumption that Mg and Mg-Sn creates stable intermetallics with Ca. The samples were either solution treated at 465°C for 96 hr and then aged in temperatures of 150°C-250°C for 1-96 hr, or thermally exposed at the as-cast condition in temperatures of 150°C-300°C for

long periods of 8-768 hr. The addition of Ca creates MgSnCa during the solidification, however in both alloys, the precipitation of  $Mg_2Sn$  and MgZn is responsible for the hardening during aging and thermal exposure.

#### 9:50 AM

Microstructural Investigations of the Mg-Sn-X and Mg-Sn-Al-X Alloy Systems: Amanda L. Bowles<sup>1</sup>; Carsten Blawert<sup>1</sup>; Norbert Hort<sup>1</sup>; Karl U. Kainer<sup>1</sup>; <sup>1</sup>GKSS Forschungszentrum, Ctr. for Magnesium Tech., Max Planck Str 1, Geesthacht 21502 Germany

In an effort to gain insight into more unusual magnesium casting alloys an investigation of the binary Mg-Sn and ternary Mg-Sn-Al systems has been undertaken. For initial investigations, permanent mould castings have been made. Various elements have been added in minor amounts to the base systems (Mg-Sn and Mg-Sn-Al) and their affect on the microstructure and hardness examined. Specimens were examined in four heat treatment conditions: as-cast (F), solution heat treated (T4), solution heat treated and aged (T6) and artificially aged only (T5) conditions. The microstructures have been examined in both a qualitative manner (optical and electron microscopy) and in a quantitative manner (XRD, EDS).

#### 10:10 AM Break

#### 10:20 AM

New Aerospace Magnesium Alloy: Paul Lyon<sup>1</sup>; <sup>1</sup>Magnesium Elektron, TSD, PO Box 23, Swinton, Manchester M27 8DD UK

Magnesium based sand casting alloys are used for aerospace applications including helicopter gearboxes and jet engine components. Over the last 20 years, key development goals for new aerospace alloys have included better elevated temperature performance combined with good corrosion resistance. Currently, the alloy with the best property envelope in this field is Elektron WE43B (Mg-Y-Nd-HRE-Zr). The castability of this alloy is however affected by a tendency to oxidation in the molten state. This requires attention to foundry detail fibest results are to be achieved. This can impact on cost. Magnesium Elektron have developed a new Magnesium alloy, with significantly improved castability, whilst maintaining a corrosion resistance and mechanical property envelope close to that of Elektron WE43b. This new alloy, currently known as Elektron X, is compared and contrasted with existing Magnesium casting alloys.

#### 10:40 AM

Computational Thermodynamics and Experimental Investigation of Mg-Al-Ca System: Yu Zhong¹; Jorge O. Sofo²; Zi-Kui Liu³; ¹Pennsylvania State University, Matls. Sci. & Engrg., 107 Steidle Bldg., Univ. Park, PA 16802 USA; ²Pennsylvania State University, Matls. Simulation Ctr., Univ. Park, PA 16802 USA; ³Pennsyvania State University, Matls. Sci. & Engrg., 209 Steidle Bldg., Univ. Park, PA 16802 USA

The laves phases in the Mg-Al-Ca ternary system are the key phases to improve the creep properties at elevated temperatures (>150°C) of Mg-based alloys. Three laves phases i.e. C14, C15 and C36 are investigated by using the Computational Thermodynamics/First-Principles calculations/experiments combined approaches. Laves phases in Mg-Al-Ca system are modeled as solution phases: (Mg,Al)2Ca. The solubility range of each laves phase is investigated. The ternary Mg-Al-Ca thermodynamic database is thus constructed and used to understand the microstructures and phase relationship of Mg-based alloys. Scheil simulations and equilibrium calculations are performed for the solidification process of the alloys and compared with experimental observations.

# 11:00 AM

The Portevin-Le Chatelier Effect and Creep Behaviour in a Mg-Ca-Zn-Zr Alloy: Suming Zhu<sup>1</sup>; Xiang Gao<sup>1</sup>; Jian-Feng Nie<sup>1</sup>; <sup>1</sup>Monash University, Sch. of Physics & Matls. Engrg., Victoria 3800 Australia

The tensile properties and creep behaviour of Mg-1Ca-0.5Zn-0.6Zr (wt.%) alloy have been studied. Serrated flow (the Portevin-Le Chatelier effect) was observed when the alloy was tensile-tested in an intermediate temperature range (150-200°C). Static strain ageing effect and negative strain rate sensitivity suggested that the serrated flow was related to dynamic strain ageing (DSA) caused by the interaction between dislocations and solute Ca atoms. In creep, the alloy exhibited periodical strain bursts at 150°C. Over-ageing treatment was shown to eliminate the occurrence of strain bursts. The creep deformation mechanism of the alloy was discussed in relation to the DSA effect.

# 11:20 AM

Computational Thermodynamic Modeling of the Al-Mg-Na System: Shengjun Zhang<sup>1</sup>; <sup>1</sup>Pennsylvania State University, Dept. Matl. Sci. & Tech., 107 Steidle Bldg., State College, PA 16801 USA

The binary Al-Na and Mg-Na systems were modeled by computational thermodynamics using the Calphad approach. Self-consistent thermodynamic parameters of the binary systems were obtained. Combined with the Al-Mg modeling in the literature with gas phase adding, the phase equilibria of the ternary system were calculated using Thermo-Calc software. Isothermal and isopleth sections of the phase diagram and the projection of the liqudus surface were presented. This present work contributes to the thermodynamic database of aluminum and magnesium alloy systems and can be included in the study of the impurity effects on processing of aluminum and magnesium alloy systems.

# Metals for the Future: Processing and Bio-Materials

Sponsored by: TMS,

Program Organizers: Manfred Wuttig, University of Maryland, Department of Materials & Nuclear Engineering, College Park, MD 20742-2115 USA; Sreeramamurthy Ankem, University of Maryland, Department of Material & Nuclear Engineering, College Park, MD 20742-2115 USA

Thursday AM Room: 215

March 18, 2004 Location: Charlotte Convention Center

Session Chair: S. Ankem, University of Maryland, Dept. of Matl. & Nuclear Engrg., College Park, MD 20742-2115 USA

### 8:30 AM Opening Remarks by S. Ankem

#### 8:40 AM Invited

Metallic Dental Implants: A Review: Sarit B. Bhaduri<sup>1</sup>; Sutapa Bhaduri<sup>1</sup>; Murali G. Kutty<sup>1</sup>; <sup>1</sup>Clemson University, Sch. of Matls. Sci. & Engrg., 110 Olin Hall, Clemson, SC 29634 USA

The dental implants form a significant share of the rapidly growing medical device market. Among the various implants, the dental implants traditionally enjoyed a high success rate. This review will begin with a brief introduction to the historical perspectives leading to discovery of such implants in Sweden. This will be followed by various classifications of implants and the distinguishing features of each class. The design and materials related issues will be a major portion of the talk. While these implants are traditionally manufactured from titanium, it is important to understand the phenomenon of "Osseointegration" (bonding of bone to the implants). Since osseointegration is a surface phenomenon, it is important to understand how the surface chemistry, morphology and the presence of a coating affect osseointegration. Various processes to obtain the desired surface features will be discussed. The presentation will conclude with some of our results in obtaining the desired surface features.

#### 9:10 AM Invited

Understanding Processing-Microstructure-Property Relationships of High-Temperature Structural Alloys Through Grain Boundary Engineering: C. J. Boehler<sup>1</sup>; S. Civelekoglu<sup>1</sup>; N. Eisinger<sup>2</sup>; J. F. Bingert<sup>3</sup>; <sup>1</sup>Alfred University, Sch. of Ceram. Engrg. & Matls. Sci., 2 Pine St., Alfred, NY 14802 USA; <sup>2</sup>Special Metals Corporation, Huntington, WV USA; <sup>3</sup>Los Alamos National Laboratory, Los Alamos, NM USA

One goal of this NSF CAREER program (DMR-0134789) is to evaluate the potential of grain boundary engineering for high-temperature structural alloys, including Ni-based superalloys and Ti2AlNb intermetallics. The program involves processing and evaluating microstructures, measuring the grain boundary character distribution (GBCD), performing mechanical testing, and modeling the effects of GBCD on mechanical behavior. Emphasis has been placed on developing a processing methodology which can be used to enhance mechanical behavior and in particular creep resistance. From electron backscattered diffraction (EBSD) analysis, the GBCD of the orthorhombic (O) and body-centered-cubic (BCC) structures of Ti-Al-Nb alloys as well as the FCC-based INCONEL alloy 718 will be presented. For the first time the twin-related O-phase variant interfacial planes, which formed from either the HCP(a2)-O or BCC-O transformation, were quantified for Ti2AlNb alloys. The preferred O-variant boundaries from the HCP-O transformation were near {110} or {130}, while the preferred O-variant boundaries from the BCC-O transformation were near {221}.

# 9:40 AM Invited

The Effects of Passivation Layers and Film Thickness on the Mechanical Behavior of Freestanding Electroplated Cu Thin Films with Constant Microstructure: Joost Johan Vlassak<sup>1</sup>;

<sup>1</sup>Harvard University, DEAS, 311 Pierce Hall, 29 Oxford St., Cambridge, MA 02138 USA

The goal of this paper is to investigate the effects of film thickness and the presence of a passivation layer on the mechanical behavior of electroplated Cu films. Both dislocation dynamics and strain-gradient plasticity models suggest that these factors play important roles in thin film plasticity. To study the effect of passivating layers, freestanding Cu membranes were prepared using silicon micromachining techniques. Some of these membranes were passivated by depositing Ti films with thicknesses ranging from 20 nm to 50 nm on both sides of the membrane. The effect of film thickness was evaluated by preparing freestanding films with varying thickness but constant microstructure, both with and without Ti passivation. The stress-strain curves of the freestanding Cu films were evaluated using the plane-strain bulge test technique. The grain structure and crystallographic texture of the Cu films were determined using EBSD, the dislocation structure through TEM. Yield stress, Young's modulus, residual stress, and work hardening behavior of the films are correlated with film microstructure and thickness.

#### 10:10 AM Break

#### 10:25 AM Invited

Metals for the Future: Environmentally Benign Pb-Free Solder Alloys: Nik Chawla<sup>1</sup>; <sup>1</sup>Arizona State University, Dept. of Chem. & Matls. Engrg., Ira A. Fulton Sch. of Engrg., Tempe, AZ 85287 USA

Solders are an integral part of electronic packaging. Recently, there has been a significant drive to replace Pb-Sn solders with Pb-free, environmentally-benign solders. Given the widespread use of Pb-Sn solder in the manufacture and assembly of circuit boards, the development and reliability of new Pb-free solders is crucial for the successful substitution of these materials in the electronics industry. In this talk an overview of the thermomechanical behavior and microstructure in Pb-free solders, in bulk form and at small length scales, will be presented. Experiments coupled with microstructure-based simulations have been conducted to further the understanding of deformation in these materials. The challenges and opportunities for metals research in this arena will be explored and discussed.

### 10:55 AM Invited

The New Renaissance of Biometallic Implants: Otto C. Wilson<sup>1</sup>; <sup>1</sup>Catholic University, BONE/CRAB Lab., Dept. of Biomed. Engrg., Washington, DC USA

Metallic implants have historically served as inactive, structural support systems to repair hard tissue damage. However, a number of advances in bioinorganic chemistry and surface probe techniques have uncovered a whole new world of applications for biometallic implants that range from macroscale to nanoscale implants. New developments in surface modification have been used to transform traditionally inert metal implant surfaces into bioactive surfaces for greatly enhanced integration into the body. The most versatile coatings in this genre include calcium phosphate based minerals (hydroxyapatite), silica based minerals (Bioglass) and even metal oxidation products such as TiO2 which exhibit unique bone bonding behaviors. Nanoscale biometallic implants for treatment of disorders at the cellular and sub cellular level are being developed based on the integral role of metal ions in biological processes such as protein function. An overview of these technologies with respect to current and future advances in metal based orthopedic and vascular implants, shape memory alloy MEMs devices for the assembly of tissue engineering scaffolds, and magnetic nanoparticles for controlled cellular interactions will be presented in this talk.

11:25 AM Panel Discussion with H. Rack, B. B. Rath, B. MacDonald

# Multiphase Phenomena in Materials Processing: Session III

Sponsored by: Extraction & Processing Division, Light Metals Division, Materials Processing and Manufacturing Division, EPD-Process Fundamentals Committee, MPMD/EPD-Process Modeling Analysis & Control Committee, MPMD-Solidification Committee Program Organizers: Ben Q. Li, Washington State University, School of Mechanical and Materials Engineering, Pullman, WA 99164-2920 USA; Stavros A. Argyropoulos, University of Toronto, Department of Materials Science and Engineering, Toronto, Ontario M5S 3E4 Canada; Christoph Beckermann, University of Iowa, Department of Mechanical Engineering, Iowa City, IA 52242 USA; Bob Dax, Concurrent Technologies Corporation, Pittsburgh, PA 15219 USA; Hani Henein, University of Alberta, Edmonton, AB T6G 2G6 Canada; Adrian S. Sabau, Oak Ridge National Laboratory, MS-602, Oak Ridge, TN 37831-6083 USA; Brian G. Thomas, University of Illinois, Department of Mechanical and Industrial Engineering, Urbana, IL 61801 USA; Srinath Viswanathan, Sandia National Laboratories, Albuquerque, NM 87185-1134 USA

Thursday AM Room: 218B

March 18, 2004 Location: Charlotte Convention Center

Session Chairs: Hani Henein, University of Alberta, Dept. of Chem. & Matls. Engrg., Edmonton, Alberta T6G 2G6 Canada; Adrian S. Sabau, Oak Ridge National Laboratory, Dept. 1835, Oak Ridge, TN 37831-6083 USA

#### 8:30 AM

Effect of Process Variables on Droplet Heat Transfer: Hani Henein<sup>1</sup>; <sup>1</sup>University of Alberta, Advd. Matls. & Procg. Lab., Dept. of Chem. & Matls. Engrg., Edmonton, Alberta T6G 2G6 Canada

Heat transfer between droplets/particles and a gas phase plays an important role in the transport of numerous materials processing operations. These include rapid solidification operations such as gas atomization and spray forming, as well as chemical systems such flash furnaces. Chemical reaction rates and solidification are dependent on the rate of gas-particle or gas-droplet heat transport. Using a heat transport model validated using single fluid atomization of molten droplets; the effect of process variables on heat losses from droplets was examined. In this work, the effect of type of gas, droplet size, gas temperature, gas-droplet relative velocity on the heat transport from AA6061 droplets was examined. The most critical of these process variables to heat transfer is identified and will be presented.

#### 8:50 AM

Separation Characteristics of Gas-Solid Flow in U-Beam Separator: *Haigang Wang*<sup>1</sup>; *S. Liu*<sup>1</sup>; Fan Jiang<sup>1</sup>; <sup>1</sup>Chinese Academy of Sciences, Inst. of Engrg. Thermophysics, PO Box 2706, Beijing, Beijing 100080 China

It is difficult to model 3D turbulent flows of a gas containing suspended solid particles through U-beam separators of complex geometry. In this paper, the complex multiphase turbulent flow in U-beam separators is simulated using the standard k-e, RNG k-e and Reynolds stress equation models (DSM) respectively. The gas-phase transport equations coupled with the gas-particle interactions are modified, based on the DSM turbulent models to handle the interaction between the gas and particles, which accounts for both the enhancement and damping of the turbulent energy by the particles. To account the effect of the stochastic characteristic of the instantaneous gas velocity on the particles, the improved Lagrangian stochastic model based on the Reynolds stress was adopted, which attributed to the successful prediction of the turbulence inhomogeniety, turbulence anisotropy, and particle crossing-trajectories effect. The collisions between the particles are also considered in the Hard-Sphere model. To treat the particle-wall collision, the influence of the roughness of the wall on the motion of the solid particles is taken into consideration by imposing random collision angles. To observe the effects of different turbulent models, the flows in a 90° bend with square cross section are simulated firstly. The results are compared with experimental data, which shows that the DSM model is superior to the other two models. It clearly predicts the anisotropic behavior of the Reynolds stresses and the distribution of the velocity in the U-beam separator. Numerical calculations of threedimensional gas-particle flow through a separator with four rows of Ubeam elements show that the particles coarser than 50 mm are mostly separated in the first two rows, particles between 20-50 mm are more likely separated in the third and fourth rows, but with less total efficiency. The collection efficiency increases with the number of U-beam elements, but with raised pressure drop too. Although initially at same starting position, the trajectories of particles of different sizes are different. The results show that the turbulence intensity strongly affects the path of the particle. The calculated results show that the particle separation also rely on particle density, size and free stream velocity. To optimize the effect of a U-beam separator, the free stream velocity and the number of U-beam element should be considered jointly.

#### 9:10 AM

Multiphase Transitions in Metals Being Electrochemically Deposited: Oleg B. Girin<sup>1</sup>; <sup>1</sup>Ukrainian State University of Chemical Engineering, Dept. of Matls. Sci., Pr. Gagarina, 8, Dnipropetrovsk 49005 Ukraine

There has been experimentally found and theoretically confirmed a change in the aggregate state of the metals being electrochemically deposited wherein while a metal is being electrodeposited on a solid cathode in an aqueous medium, a super-cooled metal liquid is formed that solidifies at the deposition temperature. In general the polymorphous metal being electrodeposited passes in succession through the following phases: metal liquid, intermediate solid modification, and stable solid phase. The fact that in the process of their electrochemical deposition the metals pass via a stage of their liquid state is confirmed by the regular changes of their microstructure, substructure, structural state, structural inhomogeneity and defects in their crystal-line structure with the supercooling degree being increased during their electrodeposition. This research project is financed by the Ministry of Education and Science of Ukraine, R&D project No. 0102U001953.

#### 9:30 AM

A Study of Steel Scrap Movement: Diancai Guo<sup>1</sup>; <sup>1</sup>McMaster University, Steel Rsch. Ctr., Hamilton, Ontario L8S 4L7 Canada

Uneven movement of scrap during melting in an Electric Arc Furnace causes operation problems; cave-ins interrupt electric power input. The movement also influences the radiation heat loss to water-cooled side panels and roof. An apparatus has been built to simulate the flow of scrap that may be interlocked. It has been observed that flow starts at the point where the suspended length of the pile bottom reaches the average scrap size, and proceeds in the form of cave-ins, but scrap pieces slide with each other as ordinary granules. After a cave-in, the pile angle usually remains much larger than the normally observed angle of repose. The internal stress of a partially suspended scrap pile has been analyzed, and the equivalent cohesion due to interlocking estimated. A numerical model has been developed to simulate the scrap flow. Simulated results agree reasonably with observed phenomena.

# 9:50 AM Break

#### 10:05 AM Cancelled

A Multiphase Solution Algorithm for Microporosity Prediction During Casting

#### 10:25 AM

**Detachment of Bubbles from Their Nucleation Sites**: László I. Kiss¹; Sándor Poncsák¹; Alicia Liedtke¹; Verena Mackowiak¹; ¹Université du Québec, Ctr. Universitaire de Recherche sur l'Aluminium, 555 boul. de l'Université, Chicoutimi, Québec G7H 2B1 Canada

Bubbles play a very important role in different metallurgical applications like in electrowinning. During heterogeneous nucleation, the maximal size of the bubbles growing at the nucleation sites as well as the nucleation frequency is determined by the so-called detachment condition. Detachment occurs when the external forces acting on the bubble exceed the retaining forces along the solid-gas-liquid triple interface line. The phenomenon depends strongly on the shape and orientation of the solid surface and on the nature and strength of the external buoyancy and drag forces. In the present study the detachment conditions of bubbles from downward facing horizontal and inclined plates were studied experimentally under the effect of gravitational and hydrodynamic forces. The results show the deformation of the bubbles under the effect of the external forces and the detachment conditions as function of the bubble volume.

#### 10:45 AM

Mechanisms and Diffusional Kinetics of the Hard Chromizing Process on Carbon Steels: *Jyh-Wei Lee¹*; Jenq Gong Duh²; ¹Tung Nan Institute of Technology, Dept. Mech. Engrg., #152, Sec. 3, Pei-Shen Rd., Shen-Ken, Taipei Co. Taiwan; ²National Tsing Hua University, Dept. Matls. Sci. & Engrg., #101, Sec. 2, Kuang-Fu Rd., Hsin Chu Taiwan

Hard chromizing process is a method for developing a surface modified coating providing wear, corrosion resistance and high temperature surface protection. Two carbon steels with 0.45 wt% and 0.95 wt% carbon contents, respectively, were chromized with pack cementation

process at 950?• for 1, 4 and 9 hours. The phase transformation and microstructure phenomena of chromized coating layer and matrix of two steels were studied with X-ray diffractometer and electron probe microanalyzer. (Cr,Fe)23C6 and (Cr,Fe)7C3 carbides and (Cr,Fe)2N1-x nitride phases were observed on the chromized surfaces. The thickness of chromized layers obeyed the parabolic rate law. The mechanism and diffusional kinetics of the chromizing process were proposed. The diffusivity of chromium in the (Cr,Fe)7C3 carbide phase was calculated using the moving boundary method.

#### 11:05 AM

A Computational Approach in Obtaining Heat Transfer Dimensionless Correlations: Blas Melissari<sup>1</sup>; Stavros A. Argyropoulos<sup>1</sup>; <sup>1</sup>University of Toronto, Dept. of Matls. Sci. & Engrg., 184 College St., Toronto, ON M5S3E4 Canada

There is a paucity of dimensionless convective heat transfer correlations applicable to fluids like liquid metals. The existing correlations cover single Prandtl number metals or at most two different Prandtl number metals. In this paper a computational approach was employed. This approach estimates the melting of solid spheres immersed in different liquid metals and under different convective conditions. The spheres are made from the same material as the liquid metal. The SIMPLER algorithm was implemented in two dimensions axi-symmetrical co-ordinates and three-dimensional Cartesian co-ordinates. Experimental validation of the dimensionless correlation was carried out in two fluids with vastly different Prandtl numbers.

#### 11:25 AM

Mathematical Modeling of Air Gap Phenomena in Squeeze Casting of Aluminum Alloys: Alfred Yu<sup>1</sup>; Naiyi Li<sup>2</sup>; Henry Hu<sup>1</sup>; University of Windsor, Mech., Auto. & Matls. Engrg., 401 Sunset Ave., Windsor, Ontario N9B 3P4 Canada; <sup>2</sup>Ford Motor Company, Mfg. Sys. Dept., Ford Rsch. Lab., Dearborn, MI 48121 USA

In the past few years, various squeeze cast aluminum components have been developed and successfully implemented in various vehicles by the automotive industry because of their superior engineering performance. However, fundamental understanding of the formation of air gap during squeeze casting processes is still very limited despite of its significant influence on the extent of heat transfer between the casting and mould. In this paper, a 3-D mathematical model has been developed to simulate phenomena of air gap between the casting and mold during squeeze casting of aluminum alloys. The model considers the effect of process parameters such as applied pressures, initial velocities and mold temperatures on the events of air gap formation. The predication indicates that the occurrence of highly enhanced heat transfer in squeeze casting of aluminum alloys primarily results from the presence of excess applied pressures.

# Nanostructured Materials for Biomedical Applications: Session VII

Sponsored by: Electronic, Magnetic & Photonic Materials Division, EMPMD-Thin Films & Interfaces Committee Program Organizers: Roger J. Narayan, Georgia Tech, School of Materials Science and Engineering, Atlanta, GA 30332-0245 USA; J. Michael Rigsbee, North Carolina State University, Department of Materials Science and Engineering, Raleigh, NC 27695-7907 USA; Xinghang Zhang, Los Alamos National Laboratory, Los Alamos, NM 87545 USA

Thursday AM Room: 219A

March 18, 2004 Location: Charlotte Convention Center

Session Chairs: Roger J. Narayan, Georgia Institute of Technology, Sch. of Matls. Sci. & Engrg., Atlanta, GA 30332-0245 USA; Marian G. McCord, North Carolina State University, Textile Engrg. Chmst. & Sci., Raleigh, NC 27695-8301 USA; Afsaneh Rabiei, North Carolina State University, Mech. & Aeros. Engrg., Raleigh, NC 27695-7910 USA

### 8:30 AM Invited

**Thin-Film Self-Assembled Nanostructured Materials**: *Andrew P. Shreve*<sup>1</sup>; Andrew M. Dattelbaum<sup>1</sup>; James H. Werner<sup>1</sup>; Meri L. Amweg<sup>2</sup>; Chanel E. Yee<sup>2</sup>; Atul N. Parikh<sup>2</sup>; <sup>1</sup>Los Alamos National Laboratory, Biosci. Div., MS G755, Los Alamos, NM 87545 USA; <sup>2</sup>University of California, Dept. of Appl. Sci., Davis, CA USA

Recent studies of thin-film self-assembled nanostructured materials will be discussed. The formation of nanocomposite thin-film silica based materials will be a special emphasis. Such materials can be formed

on solid supporting substrates from an evaporation-induced ordered surfactant phase in combination with soluble silica precursors. These structured films can be functionalized, both chemically and biochemically, using various strategies, and representative examples of such functionalization will be presented. The resulting composite materials are active thin-films with tunable responses, and some applications in sensing and molecular recognition will be described. In addition, spatial patterning using uv-processing methods is possible, and results addressing the mechanism of uv-patterning and examples of interactions of patterned functional films with biomolecular assemblies will also be presented.

#### 9:05 AM

Synthesis and Characterization of Nanostructured Inorganic-Organic Composite Biosensor Films: *Tianbao Du*<sup>1</sup>; Olusegun J. Ilegbusi<sup>1</sup>; <sup>1</sup>University of Central Florida, Dept. of Mech., Matls. & Aeros. Engrg., 4000 Univ. Blvd., Orlando, FL 32826 USA

Metal/Semiconductor (M/SC) nanoparticles immobilized in polymer matrices have generated considerable interest in recent years due to their distinct individual and cooperative properties. Such nanostructured composites have exhibited unique physicochemical, electrophysical, magnetic and optical properties. In particular, they have demonstrated potential as chemical sensors for detecting superoxide anion radicals (SOR) in biological fluids. These radicals initiate damage to tissues and biologically active substances in organisms. In this work, various semiconductor-polymer nanocomposite biosensor films for SOR are synthesized by sol-gel technique. The films are deposited from organic solutions on Pt-coated Pyrex glass substrate. They are characterized for surface morphology, chemistry, thickness, and nanocrystallite size using various advanced analytical techniques such as scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), and high-resolution transmission electron microscopy (HRTEM) aided by focused ion beam sample preparation. Preliminary results show that the solgel technique could successfully synthesize nanostructured semiconductor-polymer composites with enhanced sensitivity for detection of superoxide radicals.

#### 9:40 AM Cancelled

Bicontinuous Nanoporous Pt and Au Electrodes - Processing and Properties

#### 10:15 AM Invited

Plasma Deposition of Ultrathin Films on Nanoparticles for Bio-Sensor Applications: *Donglu Shi*<sup>1</sup>; <sup>1</sup>University of Cincinnati, Chem. & Matls. Engrg., 493 Rhodes Hall, Cincinnati, OH 45221-0012 USA

Nanoparticals are used in many applications because of their desirable bulk properties. Unfortunately, the surface of the nanoparticles is often not ideal for the particular application. The ability to deposit well-controlled thin film coatings on nanoparticles would offer a wide range of technological opportunities based on changes to both the bio and physical properties of the nanoparticals. Atomic layer controlled coatings on nanoparticles, for example, would allow them to retain their bulk properties but yield more desirable surface properties. These ultrathin coatings could act to activate, passivate or functionalize the nanoparticles to achieve both desirable bulk and surface properties. This presentation will give an overview of new surface structures by plasma deposition of ultrathin films on various nanoparticle (including nanotubes) for novel engineering applications. The unique properties required in these specific applications could be best achieved by our plasma method. One of the novel applications is in the area of biosensor applications. The fluorescent paramagnetic nanoparticles have been recently developed for various medical diagnostic and environmental applications. These nanoparticles comprise superparamagnetic cores coated or incorporated with spectrally characteristic fluorescent dyes. A thin coating of polymer or silica can be applied to these fluorescent particles to provide various functional groups for passive or covalent coupling to biologicals, such as antigens, antibodies, enzymes, or DNA/RNA hybridization. They can be used as a solid phase for various types of immunoassays and DNA/RNA hybridization probe assays, cell separation, and other diagnostic, medical, and industrial applications.

### 10:50 AM Invited

Pathogenesis of Vascular Catheter Infections as a Model of Prosthetic Implant Infection: Robert J. Sheretz<sup>1</sup>; <sup>1</sup>Wake Forest University, Sch. of Medicine, Med. Ctr. Blvd., Winston-Salem, NC 27157 USA

Prosthetic implants are used increasingly commonly in the care of patients through out the world. The most important complication interfering with their use is infection. Infection of prosthetic devices equals microorganism biofilm formation on the device plus clinical

symptoms. Central venous catheters are the best studied example of prosthetic device infection and will be used to illustrate the challenges we must face to improve the outcomes of prosthetic device implantation. Central venous catheters uniformly develop biofilm formation within three days of implantation. Only about half of these biofilms are culture positive. Of those that are culture positive the timing of initial colonization varies by catheter site: subcutaneous segment (average: 5.1 days), tip segment (8.6d), and lumen (13.1d). The greater the number of organisms on a catheter, the greater the likelihood that the catheter will have associated purulence or bloodstream infection. The risk of catheter-related bloodstream infection ranges considerably from £ 2/1000 patient days (peripheral venous catheters, peripherally inserted central catheters (PICC), cuffed central venous catheters, ports), 10/1000 patient days (arterial and Swan-Ganz catheters), to 30-50/1000 patient days (multilumen, hemodialysis). Intrinsic factors that affect the risk of vascular catheter infection include host factors, type of organism, catheter material, and the manufacturing process. Extrinsic factors that can affect the risk of infection primarily involve antiseptic technique such as skin preparation, the use of maximum sterile barriers, and education. New strategies to reduce the risk of catheter-related bloodstream infection target both the internal and external surface of the catheter including anti-infective coatings and anti-infective flush solutions. The importance of these findings to the prevention of infection involving other prosthetic devices will be discussed.

# Solid and Aqueous Wastes from Non-Ferrous Metal Industry: Session II

Sponsored by: Extraction & Processing Division, EPD-Waste Treatment & Minimization Committee

Program Organizers: Junji Shibata, Kansai University, Department of Chemical Engineering, Osaka 564-8680 Japan; Edgar E. Vidal, Colorado School of Mines, Golden, CO 80401-1887 USA

Thursday AM Room: 214

March 18, 2004 Location: Charlotte Convention Center

Session Chairs: Hideki Yamamoto, Kansai University, Dept. of Chem. Engrg. Japan; Edgar E. Vidal, Colorado School of Mines, Dept. of Metallurgl. & Matls. Engrg., Golden, CO 80401-1887 USA

#### 8:30 AM Invited

Selection of Ion-Exchange Resins Suitable for Removing Copper from Aqueous Wastes Generated During Semiconductor Processing Operations: William Ewing<sup>1</sup>; Fanny Darmawan<sup>1</sup>; Fiona M. Doyle<sup>1</sup>; James W. Evans<sup>1</sup>; <sup>1</sup>University of California, Matls. Sci. & Engrg., 210 Hearst Mining Bldg. #1760, Berkeley, CA 94720-1760

Copper is increasingly being adopted for interconnects in semiconductor devices. The aqueous processing techniques used in device manufacture generate copper-bearing wastes, such as spent electrolyte from electroplating, electroplating rinse water, and CMP waste streams. We are examining the use of ion exchange and electrowinning as a means of recovering copper from these streams within the processing plant, to allow recycling of process water and minimize hazardous wastes. Various resins have been tested for their affinity for copper in the presence of plating additives and other organic complexing agents. While chelating resins have a strong affinity for copper, their elution can be problematic. Carboxylate resins do not appear to be capable of removing copper to sufficiently low concentrations. Sulfonate resins, however, appear to be promising, provided there are not high concentrations of competing cations.

### 9:00 AM Invited

Stability of Hazardous Heavy Metal Waste by Modified Belite Cement Produced from Rolling Sludge: *Ji-Whan Ahn*<sup>1</sup>; Jin-Sang Cho<sup>1</sup>; Hyung-Seok Kim<sup>1</sup>; Ki-Suk Han<sup>1</sup>; Hwan Kim<sup>2</sup>; Choon Han<sup>3</sup>; <sup>1</sup>Korea Institute of Geoscience and Mineral Resources, Matls. & Mineral Procg. Div. Korea; <sup>2</sup>Seoul National University, Sch. of Matls. Sci. & Engrg. Korea; <sup>3</sup>Kwang-Woon University, Dept. of Chem. Engrg. Korea

The Modified belite cement clinker containing  $\beta$ -C<sub>2</sub>S, C<sub>4</sub>A<sub>3</sub>S and C<sub>4</sub>AF was synthesized using industrial by-product, and the solidification/stabilization properties of hazardous heavy metal and organic matter including in industrial wastes by cement produced were investigated. For synthesis of modified belite cement clinker, the raw materials were mainly used rolling sludge, dolomite sludge generated at steel and iron making process, and phosphogypsum generated at soda lime

manufacturing process. The mixture of raw materials was sintered at 1250° for 1hr and cooled rapidly in air condition, and properties of the clinker were characterized with XRD, SEM, and EDAX. The Modified belite cement was produced mixing clinker and calcium sulfate (CaSO<sub>4</sub>). Using XRD, SEM, compressive strength and leaching test of heavy metal, hydration and solidification/stabilization properties of hazardous wastes containing heavy metal and organic matter were investigated.

#### 9:30 AM Invited

Solvent Extraction of Nickel in the Spent Electroless Nickel Plating Baths: Mikiya Tanaka<sup>1</sup>; Hirokazu Narita<sup>1</sup>; <sup>1</sup>National Institute of Advanced Industrial Science and Technology Japan

With increasing importance of electroless nickel plating technology in many fields such as electronic and automobile industries, the treatment of the spent baths is becoming a serious problem. Although the spent baths are currently treated by conventional precipitation method, a method with no sludge generation is desired. In the EPD Congress 2003, we reported the solvent extraction recovery of nickel from the spent baths by means of solvent extraction using LIX84I as an extractant. A drawback of that method was that the extraction and stripping of nickel were not fast enough to achieve high efficiencies when the continuous extractor was used. We have overcome this difficulty by finding an effective accelerating reagent added into the organic phase of LIX84I. Shaking out tests using a separatory funnel at 240 spm revealed that the extraction and stripping rates of nickel are remarkably enhanced by adding the accelerating reagent: The time to reach equilibria is more than 60 min without additive, but reduced to 10 min by the additive both in the extraction and the stripping with sulfuric acid. Detailed data on the accelerating effects will be presented.

#### 10:00 AM Break

#### 10:15 AM

Recycling Process for Tantalum and Some Other Reactive Metal Scraps: Ryosuke Matsuoka<sup>1</sup>; Kunio Mineta<sup>1</sup>; Toru H. Okabe<sup>1</sup>; <sup>1</sup>University of Tokyo, Inst. of Industrial Sci. Japan

A process of recycling tantalum from capacitor scraps using an oxidation process followed by mechanical separation and chemical treatment was investigated. This study demonstrates that sintered tantalum electrodes inside the capacitor scraps could be collected mechanically after the oxidation of the scraps in air, and high purity  ${\rm Ta}_2{\rm O}_5$  powder could be efficiently recovered after chemical treatment. The yield of tantalum from the scraps was approximately 90-92%. By reducing the tantalum oxide obtained by magnesiothermic reduction, tantalum powder with 99 mass% purity was obtained. Chlorination routes for tantalum recovery was also investigated, and the obtained tantalum or tantalum compounds were reacted with chloride scraps such as FeClx. The recycling process by utilizing chloride scrap is extended to other reactive metals (e.g. Ti, RE..).

### 10:35 AM

Novel Recovering System of Nickel in Waste Water With Solvent Extraction Technique: Yoshinobu Kawano<sup>1</sup>; Sana Takashi<sup>1</sup>; Koichiro Shiomori<sup>1</sup>; <sup>1</sup>Miyazaki University Japan

Novel recovering system of nickel in waste water was developed using solvent extraction technique. Three steps of vibro-mixer type extractors, forward extraction of nickel into the organic solution, back extraction of nickel into the aqueous solution and final purification of nickel in the aqueous solution were connected in series. Waste water was followed and treated with continuously in the system. Optimum condition of the recovering system was determined experimentally in the various operation conditions in each step.

#### 10:55 AN

Removal of Toxic Heavy Metal Ions from Wastewater with Iron-Manganese Compound: Ruilu Liang<sup>1</sup>; Eiji Kikuchi<sup>1</sup>; Hiroshi Sakamoto<sup>1</sup>; <sup>1</sup>Akita Prefectural University, Fac. of Sys. Sci. & Tech. Japan

In this paper, adsorption of cadmium, lead, arsenic and selenium ions onto iron-manganese compound adsorbent in aqueous solution was investigated. It was found that the adsorption capacity of the adsorbent is highest under the synthetic conditions: mole ratio of iron to manganese =1:1.5, reacting pH=11 and drying temperature of filter cake =70°. Based on the adsorption isotherms of Cd and Pb ions by the adsorbent, the maximum adsorption amounts were 40 mg Cd and 300 mg Pb per gram adsorbent, respectively. The metal ions were eluted from the iron-manganese compound by adding 0.5 mol/l HNO<sub>3</sub>, and the adsorption capacity of the adsorbent recovered to nearly the previous level. In addition, some fundamental aspects involved in the adsorption are also discussed.

#### 11:15 AM

Hydrometallurgical Method for Treating Special Alloys, Jewelry, Electronic and Electrotechnical Scrap: N. I. Antipov<sup>1</sup>; A. V. Tarasov<sup>1</sup>; V. M. Paretsky<sup>1</sup>; <sup>1</sup>State Research Center of Russian Federation, State Rsch. Inst. of Nonferrous Metals, 13, Acad. Korolyov St., 129515 Moscow Russia

A purely hydrometallurgical flowsheet developed in the Gintsvetmet Institute is based on the use of a versatile acidic technique for recovery of precious and non-ferrous metals into solution. This flowsheet ensures separate recovery of silver and gold, as well as commercial-grade palladium and platinum metal powders. Two alternatives are possible for manufacture of silver metal powder from silver chloride. Depending on the palladium content of solution different alternatives are possible for palladium concentration and refining. Palladium metal powder is produced by aqueous heterogeneous reaction of palladosamine with formic acid. Platinum metal powder is produced by aqueous heterogeneous reaction of ammonium hexachloroplatinate with formic acid at 90°C to 100°C. The proposed flowsheet makes it possible to reliably obtain commercial-grade products of the following quality: bullion gold containing (%%): 99.6-99.9 Au, 0.05-0.2 Ag, 0.007-0.02 Cu, 0.003-0.04 Pd, 0.003-0.005 Fe, 0.005 Pb, 0.005 Sb and 0.005 Bi; - bullion silver containing (%%):99.6-99.9 Ag, 0.07-0.3 Au, 0.01-0.03 Pd, 0.007-0.02 Cu, 0.003-0.005 Fe, 0.005 Pb, 0.005 Sb, 0.005 Bi; platinum and palladium metal powders.

# Solidification of Aluminum Alloys: Special Effects

Sponsored by: Materials Processing & Manufacturing Division, MPMD-Solidification Committee

Program Organizers: Men Glenn Chu, Alcoa Inc., Alcoa Technical Center, Alcoa Center, PA 15069 USA; Douglas A. Granger, GRAS, Inc., Murrysville, PA 15668-1332 USA; Qingyou Han, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6083 USA

Thursday AM Room: 207B/C

March 18, 2004 Location: Charlotte Convention Center

Session Chairs: Qingyou Han, Oak Ridge National Laboratory, Metals & Ceram. Div., Oak Ridge, TN 37831-6083 USA; Srinath Viswanathan, Sandia National Laboratories, Albuquerque, NM 87185-1134 USA

# 8:30 AM

Mechanisms of Grain Size Evolution During Aluminum Spray Forming: *Yaojun Lin*<sup>1</sup>; Yizhang Zhou<sup>1</sup>; Enrique J. Lavernia<sup>1</sup>; <sup>1</sup>University of California, Dept. of Chem. Engrg. & Matls. Sci., Davis, CA 95616-5294 USA

A numerical approach is implemented to analyze the evolution of grain size during spray forming 5083 Al. The evolution of grain size is investigated at the two different thicknesses of the deposit, correspond to 400 and 602°C on the deposit's surfaces. The temperature histories of individual droplets during the flight stage and during impingement onto the two aforementioned deposit's surfaces are calculated. In terms of the calculatd temperature histories, the nucleation behavior and the nuclei growth in individual droplets are computed accordingly. Based on the measured temperature history, nuclei coarsening during the solidification process of remaining liquid phase (applicable to the deposit's surface of 602°C) and grain growth during solid phase cooling are evaluated. The calculated results indicate a bimodal and a relatively uniform grain morphology, corresponding to the deposit's surfaces with the temperature of 400 and 602°C, respectively.

#### 8:50 AM

Prediction of Microstructure and Distribution of Solute in Ternary Al-Zn-Mg Alloys Designed for Cathodic Protection Applications: *Julio Alberto Juarez*<sup>1</sup>; Carlos Gonzalez<sup>1</sup>; <sup>1</sup>Universidad Nacional Autonoma de Mexico, Inst. de Investigaciones en Materiales, Circuito Exterior S/N, Cd. Universitaria, Mexico, D.F. 04510 Mexico

An analysis of the structure obtained in chill-cast Al-Zn-Mg ingots was carried out. The microstructure consisted of alpha-dendrites, tau-intermetallic in solid solution and eutectic in interdendritic regions. The electrochemical behavior of alloys in both cast and heat-treated ingots was investigated in 3% NaCl solution. Results showed that the eutectic and the intermetallic have an impact on the electrochemical efficiency of the alloys, which are designed to be used as sacrificial anodes. To correlate structure with electrochemical efficiency, the Al-Zn-Mg phase diagram for a constant concentration of Zn was analyzed together with growth temperature of phases obtained during solidifica-

tion. Then, the range of solidification front velocities was predicted, where the alpha-Al and intermetallic phases grew simultaneously. These results, together with the predicted variation with growth velocity of solute concentration in the alpha-Al and the electrochemical efficiency values were used to select an alloy which can be used as Alsacrificial anode.

#### 9:10 AM

The Effect of Casting Parameters on the Quality of Thin Gauge Foils: Murat Dündar<sup>1</sup>; Özgül Keles<sup>1</sup>; Bilal Kertý<sup>1</sup>; <sup>1</sup>Assan Aluminum, Tuzla, Istanbul Turkey

In the Aluminum Industry, wrought products with a thickness of 6-200µm are known as foils. Aluminum foil is a preferred material in the packaging industry due to its excellent electrical and heat conductivity, strength, corrosion resistance, cleanliness, compatibility with laminates, impermeability to gas and light, ease of folding, non-toxicity, etc. In today's market, a large percentage of foil production is the result of a combination of conventional ingot casting and hot rolling. The high production costs and time involved in conventional casting has led foil producers to consider continuous casting techniques, especially twin roll casting. One of the challenges of twin roll casting is the solidification process. In this study, the effects of casting parameters on the quality of foil products have been investigated using two different casters. Quality characteristics, such as number of pinholes in the foil, microstructure of the cast product, micro-macro segregation, and grain size, have been examined using mechanical, metallographic, and surface characterization techniques.

#### 9:30 AM

Effect of Mold Vibration on the Solidification Process During Die Casting of AA 356: Numan M. Abu-Dheir<sup>1</sup>; Marwan K. Khraisheh<sup>1</sup>; Kozo Saito<sup>1</sup>; <sup>1</sup>University of Kentucky, Ctr. for Mfg., Mech. Engrg. Dept., 210 CRMS Bldg., Lexington, KY 40506-0108 USA

Mechanical mold vibration using an electromagnetic shaker has been applied to the gravity die casting of AA356. The effect of vibration on the solidification process is being studied through analysis of temperature gradient in the mold. The AA356 is heated to 850°C and then poured into a steel die. The die is then vibrated at different combinations of frequency and amplitude. The mold temperature is measured and analyzed using thermocouples and high resolution images of IR camera. It is shown that the mold vibration alters the temperature profiles. This will have a significant effect on the microstructure and properties of the cast which are currently investigated.

# 9:50 AM Break

#### 10:10 AM

Correlation of Microstructure and Fluidity in Short Fiber-Aluminum Alloy Matrix Composites—A Comparison With Unreinforced Matrix Alloys: Olga B. Garbellini<sup>1</sup>; Carina N. Morando<sup>2</sup>; Hugo A. Palacio<sup>1</sup>; Heraldo Biloni<sup>1</sup>; <sup>1</sup>University Nacional del Centro de la Provincia de Buenos Aires, IFIMAT-Fac. Cs. Exactas & CICPBA, Pinto 399, Tandil B7000GHG Argentina; <sup>2</sup>University Nacional del Centro de la Provincia de Buenos Aires, IFIMAT-Fac. Cs. Exactas & SeCyT UNCPBA, Pinto 399, Tandil B7000GHG Argentina

This is a study of the fluidity in AlCuSi/Al $_2O_3$  composites at the Alrich corner. The fluidity measurements were carried out in terms of a classic foundry practice (i.e., the length the liquid metal flow in a channel packed with an alumina chopped fibers preform while solidifying). The fluidity mechanism was investigated with a focus on microstructure and the fluidity values of eutectics that complete solidification. The results of the fluidity tests indicated that the infiltrated length was best in the alloys and composites situated in the primary Si field, followed by those situated in the primary Al field and close to the the Al-Cu eutectic valley and to the Al-Si eutectic valley respectively. In all cases the results were found to be influenced by the morphology and concentration of constituent phases in the microstructure. They were compared with the results of fluidity tests in unreinforced matrix alloys. Quantitative metallography measurements are presented to substantiate such interpretations.

#### 10:30 AM

Effects of Hot Extrusion Prior to Spheroidization on Al-Si-Cu Alloys: Vjekoslav Franetovic<sup>1</sup>; Jon T. Carter<sup>1</sup>; <sup>1</sup>General Motors, R&D Ctr., Matls. & Processes Lab., MC 480-106-212, 30500 Mound Rd., Warren, MI 48090-9055 USA

The influence of prior hot extrusion of an Al-7%Si-0.5%Mg-3%Cu alloy on the subsequently spheroidized microstructure was studied. Such extrusion promoted a greater degree of spheroidization, smaller alpha globules, and higher levels of entrapped eutectic and entrapped Cu-rich phase, but no net change in copper concentration in the alpha globules (other than the entrappent). The greater degree of spheroidization

and the smaller globule size are expected to increase semi-solid formability, but the higher level of entrapped eutectic is expected to slightly reduce semi-solid formability. In samples which were T6 heat treated after spheroidization, the pre-spheroidization extrusion caused an increase of 0.5% Cu in the alpha, but no change in microhardness of either the primary alpha or the eutectic. Data are presented in the forms of optical and scanning electron micrographs, heating curves, and compositional analyses.

#### 10:50 AM

Vacuum-Sealed Aluminum Step Casting: Johnathon Capps<sup>1</sup>; Amit Suryawanshi<sup>1</sup>; Sayavur I. Bakhtiyarov<sup>1</sup>; Ruel A. Overfelt<sup>1</sup>; <sup>1</sup>Auburn University, Mech. Engrg. Dept., 202 Ross Hall, Auburn, AL 36849-5341 USA

In this paper experimental data of mold filling and solidification of aluminum alloy A356.2 in V-process casting technique are presented. A vacuum-sealed step pattern (V-process) has been used as a mold. A laboratory apparatus for a gravity filled vacuum-sealed casting was designed and built for an experimental study of the effect of some process parameters on the filling behavior of aluminum alloy in a steppattern casting. Temperature measurements and "cell-valued discretisation" method has been used to estimate contour maps of the mold filling dynamics. The position of the molten metal front is represented by isochronal lines plotted every 0.2 sec. Solidification rates of an aluminum alloy in sections of different thickness are studied and compared. The experimental results obtained in this study are compared to those predicted by prior numerical simulations.

#### 11:10 AM

Shear Behaviour of a Semi-Solid Al-Cu4.5 Wt.Pct Alloy in Relation to its Microstructure: P.-D. Grasso<sup>1</sup>; J.-M. Drezet<sup>1</sup>; J.-D. Wagnière<sup>1</sup>; M. Rappaz<sup>1</sup>; <sup>1</sup>Ecole Polytechnique Fédérale de Lausanne (EPFL), Computational Matls. Lab. (LSMX), MX-G, CH-1015 Lausanne Switzerland

The secondary creep rate for an Al-Cu4.5 wt.pct alloy in the semisolid state has been measured for different microstructures: equiaxed, columnar parallel to the shear plane and columnar perpendicular to the shear plane. These microstructures have been obtained by casting the alloy either with grain refiner to get the equiaxed structure or without to get the columnar one. In the latter case, the cooling has also been adapted in order to obtain the right direction of the columnar grains with regard to the shear plane. From these castings, a sample consisting of an hollow cylinder with a reduced section at mid-height has been machined. The heating of the sample is provided by an induction coil up to a given temperature and the application of the torsion is done by using a pneumatic motor directly fixed on the sample. Different torques and temperatures corresponding to solid fractions higher than 85% are investigated in order to study the different parameters of a classic creep Norton law. Moreover, the influence of the microstructure on the mechanical behaviour of the mushy alloy is discussed. This study was carried out within the framework of the VIR[CAST] project, in which the problem of hot tearing is addressed.

# Surfaces and Interfaces in Nanostructured Materials: Self-Organized and Biological Materials

Sponsored by: Materials Processing and Manufacturing Division, MPMD-Surface Engineering Committee

Program Organizers: Sharmila M. Mukhopadhyay, Wright State University, Department of Mechanical and Materials Engineering, Dayton, OH 45435 USA; Arvind Agarwal, Florida International University, Department of Mechanical and Materials Engineering, Miami, FL 33174 USA; Narendra B. Dahotre, University of Tennessee, Department of Materials Science & Engineering, Knoxville, TN 37932 USA; Sudipta Seal, University of Central Florida, Advanced Materials Processing and Analysis Center and Mechanical, Materials and Aerospace Engineering, Oviedo, FL 32765-7962 USA

Thursday AM Room: 217A

March 18, 2004 Location: Charlotte Convention Center

Session Chair: Sudipta Seal, University of Central Florida, Advd. Matls. Procg. & Analysis Ctr., Oviedo, FL 32765-7962 USA

# 8:30 AM

**Tribological Properties of Diamondlike Carbon-Metal Nanocomposites**: *Roger Jagdish Narayan*<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Sch. of Matls. Engrg., Rm. 361, Love Bldg., 771 Ferst St. NW, Atlanta, GA 30332-0245 USA

Diamondlike carbon (DLC) consists mainly of sp^3-bonded carbon atoms. DLC coatings possess properties close to diamond in terms of hardness, atomic smoothness, and chemical inertness. Unfortunately, DLC exhibits poor adhesion to metals and polymers. This research involves processing, characterization and modeling of DLC nanocomposite films specifically to improve adhesion and wear properties. A novel target design was adopted to incorporate noncarbon atoms into the DLC films during pulsed laser deposition. STEM-Z contrast and PEELS techniques elucidated atomic structure and bonding characteristics. Wear and adhesion tests demonstrate DLC nanocomposites possess greatly improved mechanical properties. Careful analysis of the Raman data also indicates a significant shift to shorter wavelength with the addition of metal, indicating a reduction in compressive stress. By varying the metal concentration as a function of distance from the interface, it is possible to create a functionally gradient DLC film. These nanocomposite coatings have multiple biomedical applications.

#### 8:55 AM

**DNA-Grafting as a Controlled Nano-Interface**: *Eric Geiss*<sup>1</sup>; Sejong Kim<sup>2</sup>; Fotios Papadimitrakopoulos<sup>2</sup>; Harris L. Marcus<sup>1</sup>; <sup>1</sup>University of Connecticut, Inst. of Matls. Sci., Metall. & Matls. Engrg. Dept., U3136, Storrs, CT 06269-3136 USA; <sup>2</sup>University of Connecticut, IMS Polymer Prog. & Chmst. Dept., U3136, Storrs, CT 06269-3136 USA

Recently, DNA hybridization has been increasingly adopted in materials sciences due to its capability of specific and reversible molecular recognition. These unique properties of DNA have been used for the realization of 2-D assembly of colloidal particles as a precursor to constructing 3-D photonic crystal in a layer-by-layer manner. In order to precisely understand this DNA-assisted assembly of colloidal particles we have quantitatively assessed the surface density of grafted and hybridizing accessible DNA oligomers as the controlled nano-interface on both substrate and colloidal particles. The variations of the concentration of hybridized DNA as a function of parameters such as the number of DNA base pairs, the length of spacer and the size of particle were also investigated to determine the thermal stability and the immobilization strength of colloidal particles on various surfaces.

#### 9:20 AM

Building Microstructures of Organized Carbon Nanotubes by Chemical Vapor Deposition: *Zhengjun Zhang*<sup>1</sup>; Ye Zhao<sup>1</sup>; Ya Zhou<sup>1</sup>; <sup>1</sup>Tsinghua University, Dept. of Matls. Sci. & Engrg., Beijing 100084 China

Chemical vapor deposition (CVD) using ferrocene (Fe(C5H5)2) and xylene (C8H10) is an economic way to grow carbon nanotubes and is frequently employed to fabricate, and to investigate the growth mechanism of nanotubes on planar substrates. The growth of carbon nanotubes by this approach, as we observed, showed interesting selforganization behaviors at early growth stages, which is closely related to the ratio of catalyst over carbon. Investigation on the very early deposition stages of this CVD means demonstrated that, the selforganization of carbon nanotubes is determined by the way that the catalyst particles adhere to the substrate surface, and the growth kinetics following. This provides ways to control the growth and selforganization of carbon nanotubes. For instance, one might control the adhesion of catalyst particles at the very early deposition stage or the growth kinetics shortly afterwards, to tune the self-organization of nanotubes to build microstructures of organized carbon nanotubes. By adjusting the growth kinetics of carbon nanotubes at the early deposition stages, we successfully fabricated different microstructures of carbon nanotubes on planar silicon substrates.

#### 9:45 AM

HA/DLC Nanocomposite Coatings for Improved Bioactivity and Biocompatibility of Orthopaedic Prostheses: Bryan F. Bell<sup>1</sup>; Roger J. Narayan<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Sch. of Matls. Engrg., Rm. 361, Love Bldg., Atlanta, GA 30332-0245 USA

Bioactive coatings made of hydroxyapatite (HA) mimic the mineral composition of natural bone. Unfortunately, problems with adhesion, poor chemical and mechanical integrity, and incomplete bone ingrowth limit the use of current hydroxyapatite surfaces. We have developed a novel technique using pulsed laser deposition to produce bioactive hydroxyapatite surfaces on a diamondlike carbon (DLC) interlayer. DLC is an amorphous, hydrogen-free, and primarily sp3-bonded form of carbon that exhibits exceptional biocompatibility, wear and corrosion resistance, and mechanical properties. The underlying titanium substrate is first coated with silver-doped DLC using pulsed laser deposition (PLD). The silver dopant aids in adhesion and conveys antimicrobial properties to DLC. The DLC surface is then coated with HA to form the final bilayer material. The films were characterized using SEM, TEM, XRD, Raman spectroscopy, and me-

chanical testing. HA/DLC bilayers are promising for use in several different orthopaedic implant designs.

# The Role of Grain Boundaries in Material Design: Simulation of Grain Boundary Effects of Properties

Sponsored by: Materials Processing and Manufacturing Division, ASM/MSCTS-Texture & Anisotropy Committee, MPMD-Computational Materials Science & Engineering-(Jt. ASM-MSCTS) Program Organizers: Brent L. Adams, Brigham Young University, Department of Mechanical Engineering, Provo, UT 84602-0001 USA; Thomas R. Bieler, Michigan State University, Department of Chemical Engineering and Materials Science, East Lansing, MI 48824-1226 USA

Thursday AM Room: 218A

March 18, 2004 Location: Charlotte Convention Center

Session Chairs: Christopher A. Schuh, Massachusetts Institute of Technology, Dept. of Matls. Sci. & Engrg., Cambridge, MA 02139 USA; Thomas A. Mason, Los Alamos National Laboratory, Matls. Sci. & Tech., Los Alamos, NM 87545 USA

# $8\colon\!\!30$ AM $\,$ A.D. Rollett Texture Optimization via Grain Growth and Recrystallization

#### 8:55 AM Invited

Insights on Deformation Modes in Hexagonal Metals and Constitutive Modeling: *Thomas A. Mason*<sup>1</sup>; Benjamin L. Hansen<sup>1</sup>; Benjamin L. Henrie<sup>1</sup>; George C. Kaschner<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory, Matls. Sci. & Tech., MS G755, Los Alamos, NM 87545 USA

The classic works of Kocks, Argon, Ashby and Mecking have used a constitutive model based on internal state variables to model the plastic response of many materials. Difficulty arises when this method is extended to lower symmetry metals where a number of deformation modes contribute to the strain accommodation. Additionally, the activities of the individual modes are strain-rate and temperature dependent and are strongly influenced by the crystallographic texture. This presentation will describe an effort to first quantify and then predict the deformation mode activities in textured hexagonal metals for a variety of deformation rates and temperatures. This is work comprises efforts in quantification of twin area fractions, connection of this information to hardening behaviors and finally to development of a robust, expanded capability to deal with hardening and softening behaviors more complex than the traditional, scalar Voce law.

#### 9:20 AM

Atomic Modeling of the Effects of C and H Impurities on the Grain Boundary Fracture in bcc Fe: Margarita Ruda<sup>1</sup>; Diana Farkas<sup>2</sup>; <sup>1</sup>Centro Atomico Bariloche, CNEA, Bariloche, Rio Negro Argentina; <sup>2</sup>Virginia Tech, Matls. Sci. & Engrg., Blacksburg, VA 24061 USA

We investigated the fracture behavior of a symmetrical tilt [001] (310) grain boundary in bcc iron using atomistic simulation techniques. The effects of interstitial impurities including H and C on grain boundary cohesion and fracture behavior were studied using empirical interatomic potentials. Hydrogen was found to decrease grain boundary cohesion and promote grain boundary fracture, while carbon has the opposite effect.

#### 9:40 AM

Modeling Dislocation Interaction With Grain Boundaries Using Dislocation Dynamics: Tariq Khraishi<sup>1</sup>; Yu-Lin Shen<sup>1</sup>; <sup>1</sup>University of New Mexico, Mech. Engrg. Dept., MSC01-1150, Albuquerque, NM 87131 USA

In this work, some preliminary attempts at modeling the dynamic interaction of dislocations with grain boundaries are presented. The modeling technique is that of newly developed dislocation dynamics. The results show interesting micromechanical features of the elastic fields of the boundaries as well as the salient features of their interaction with dislocations. Most importantly, the effect of grain boundaries on the strengthening of crystals is exhibited in a parametric study.

#### 10:00 AM Break

# 10:20 AM Invited

Scaling Laws for Grain Boundary Networks: Megan Frary<sup>1</sup>; Christopher A. Schuh<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology, Dept. of Matls. Sci. & Engrg., 77 Mass. Ave., Rm. 8-211, Cambridge, MA 02139 USA

Grain boundary networks have frequently been described using concepts from percolation theory, although their topologies are highly nonrandom due to crystallographic constraints. Recent works have identified numerical values for the percolation thresholds of various grain boundary networks, but this value represents only the very beginning of a comprehensive theory of network topology. Here we consider several other aspects of the grain boundary percolation problem using Monte Carlo simulations, including the distribution of boundary cluster sizes, their radii of gyration, and the fractal character of the network. In particular, we focus upon the set of universal scaling laws that link these descriptors, and which are expected to be independent of the shape of the lattice. We compare the scaling laws obeyed for nonrandom grain boundary networks to the "universal" scaling laws usually applicable to random networks, and discuss how crystallography influences these relationships. Finally, we consider the practical relevance of scaling relationships in materials design, especially with regard to small-scale structures.

#### 10:45 AM

Capturing the Role Grain Boundaries in Microstructure-Based Finite Element Models: W. A. Counts<sup>1</sup>; C. C. Battaile<sup>1</sup>; M. V. Braginsky<sup>1</sup>; T. E. Buchheit<sup>1</sup>; <sup>1</sup>Sandia National Laboratories, Albuquerque, NM USA

A microstructure-based finite element model that does not incorporate appropriate length scales cannot capture important experimentally observed phenomena linked to material microstructure. Examples include: grain boundary strengthening and deformation evolution of microstructure that leads to the development of subgrains. To overcome this deficiency, two different approaches have been developed and incorporated into a microstructure-based polycrystal plasticity finite element model: (1) a grain boundary offset model, and (2) a nonlocal integral model. In the grain boundary offset model, the length scale is the result of ad-hoc strengthening of the material near the grain boundary. Conversely, in the nonlocal integral model, a length scale falls out of an integral approximation of the strain gradient and the associated geometrically necessary dislocations (GND's). The results of these two approaches will be compared to each other and to experiments to determine if either or both approaches can provide an accurate and computationally viable method to capture the role of grain boundaries in polycrystalline materials. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States DOE under Contract DE-ACO4-94-AL85000.

#### 11:05 AM Invited

Software of Simulation of Oxidation Processes: Jerzy A. Szpunar<sup>1</sup>; Hualong Li<sup>2</sup>; <sup>1</sup>McGill University, Dept. Matls. Sci. & Engrg., 3610 Univ. St., Montreal, Quebec H3A 2B2 Canada; <sup>2</sup>ResMat Corp., 3637 Univ. St., Montreal, Quebec H3A 2B3 Canada

A discrete simulation methodology has been developed that incorporates many structural characteristics of polycrystalline material properties, such as, texture, grain boundary, microstructure, phase composition, chemical composition, stored energy, and residential stress. The computer models developed to study oxidation process is based on quantitative description of oxide and substrate structure. That description allows to simulate the transport of metal and oxygen ions along interfaces and bulk portion of materials. The proposed model help researchers and engineers to understand physical mechanism of oxidation, predict material behaviour, and optimize material processing and properties. In this paper, we will present the results of simulation results of oxidation process on different substrate of Zr-Nb alloys, which are used for manufacturing the pressure tube in CANDU nuclear reactors. The effects of substrate texture, microstructure, grain boundary, and beta phase distribution on oxidation kinetics and hydrogen permeation will be demonstrated.

#### 11:30 AM

**Software of Simulation of Recrystallization Process**: *Hualong Li*<sup>1</sup>; JongTae Park<sup>2</sup>; Jerzy A. Szpunar<sup>3</sup>; <sup>1</sup>ResMat Corp., 3637 Univ. St., Montreal, Quebec H3A 2B3 Canada; <sup>2</sup>POSCO, Tech. Rsch. Lab., PO Box 36, Pohang, Kyoungbuk Korea; <sup>3</sup>McGill University, 3600 Univ. St., Montreal, Quebec H3A 2B2 Canada

A discrete simulation methodology has been developed that incorporates various structural characteristics of polycrystalline materials such as, texture, grain boundary, microstructure, phase composition, chemical composition, stored elastic energy, and residential stress. The computer models developed based on this microstructural description of polycrystalline materials have been used to simulate the processes of oxidation, grain growth, recrystallization, and diffusion. These models can help researchers and engineers to understand physical mechanism, predict material behaviour, and optimize material processing

and properties. In this paper, we will present the results of simulation of recrystallization process in 1%Si and 2% Si steel. The deformation texture and microstructure, stored energy and the microstructure prior to deformation are among the major factors in determining the recrystallization texture, and grain growth and kinetics of structure transformation. The comparison of simulation with experimental results is presented.

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