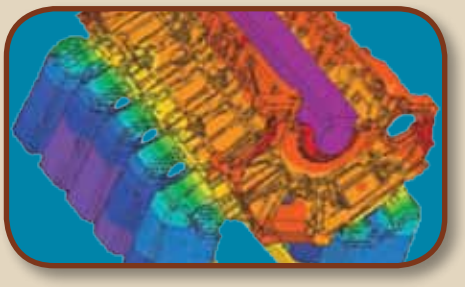
# TMS ICME

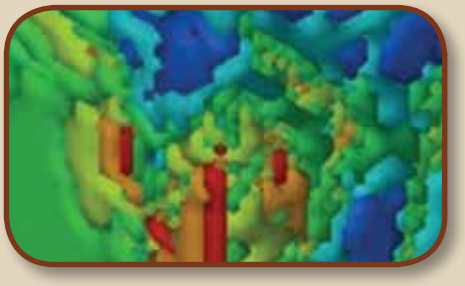
MANUFACTURING

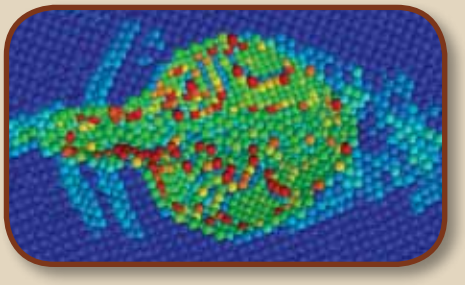
DESIGN MATERIALS

## 2nd World Congress on Integrated Computational Materials Engineering

**July 7-11, 2013**
**Salt Lake Marriott Downtown at City Creek**
**Salt Lake City, Utah, USA**







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# PROGRAM & ABSTRACTS

# SCHEDULE AT-A-GLANCE

**Sunday, July 7**

| | | |
|---|---|---|
| Registration | 6:00 p.m. to 9:00 p.m. | Ballroom Pre-function Area |
| Opening Session | 8:00 p.m. to 9:40 p.m. | Ballroom D&E |
| Welcome Reception | 10 p.m. to midnight | Ballroom F |

**Monday, July 8**

| | | |
|---|---|---|
| Registration | 7:30 a.m. to 4:30 p.m.; 7:30 p.m. to 8:30 p.m. | Ballroom Pre-function Area |
| Session: ICME Success Stories and Applications | 8:00 a.m. to 9:55 a.m. | Ballroom D&E |
| Exhibition Set-up | 9:00 a.m. to noon | Ballroom AB&C |
| Session: ICME Applications: Lightweight Materials | 10:15 a.m. to 11:35 a.m. | Ballroom D |
| Session: ICME Applications: Composites | 10:15 a.m. to 11:35 a.m. | Ballroom E |
| Lunch | 11:35 a.m. to 1:35 p.m. | On Your Own |
| Session: ICME Applications: Non-Ferrous | 1:35 p.m. to 4:15 p.m. | Ballroom D |
| Session: ICME Applications: Ferrous | 1:35 p.m. to 4:15 p.m. | Ballroom E |
| Exhibition | 2:00 p.m. to 3:30 p.m.; 8:00 p.m. to 10:00 p.m. | Ballroom AB&C |
| Poster Session I and Reception | 8:00 p.m. to 10:00 p.m. | Ballroom AB&C |

**Tuesday, July 9**

| | | |
|---|---|---|
| Registration | 7:30 a.m. to 4:30 p.m.; 7:30 p.m. to 8:30 p.m. | Ballroom Pre-function Area |
| Session: Process Optimization | 8:20 a.m. to 11:20 a.m. | Ballroom D |
| Session: Materials Data for ICME | 8:00 a.m. to 11:40 a.m. | Ballroom E |
| Exhibition | 9:00 a.m. to 10:30 a.m.; 3:00 p.m. to 4:30 p.m.; 8:00 p.m. to 10:00 p.m. | Ballroom AB&C |
| Lunch | 11:40 a.m. to 2:00 p.m. | On Your Own |
| Session: Materials Data and Tools | 2:00 p.m. to 4:45 p.m. | Ballroom D&E |
| Poster Session II and Reception | 8:00 p.m. to 10:00 p.m. | Ballroom AB&C |

**Wednesday, July 10**

| | | |
|---|---|---|
| Registration | 7:30 a.m. to 5:30 p.m. | Ballroom Pre-function Area |
| Exhibition | 8:30 a.m. to 11:30 a.m.; 3:30 p.m. to 5:00 p.m. | Ballroom AB&C |
| ICME Building Blocks: Opening Session | 8:00 a.m. to 9:10 a.m. | Ballroom D&E |
| Session: ICME Building Blocks: Experimental Tools | 9:30 a.m. to 12:30 p.m. | Ballroom D |
| Session: ICME Building Blocks: First Principles and Atomistic Tools | 9:30 a.m. to 12:50 p.m. | Ballroom E |
| Lunch | 12:50 p.m. to 2:30 p.m. | On Your Own |
| Session: ICME Building Blocks: Computational Thermodynamics and Kinetics | 2:30 p.m. to 5:50 p.m. | Ballroom D |
| Session: ICME Building Blocks: Process and Performance Modeling | 2:30 p.m. to 5:30 p.m. | Ballroom E |
| Exhibition Dismantle | 5:00 p.m. to 8:00 p.m. | Ballroom AB&C |
| Congress Dinner | 8:00 p.m. to 10:00 p.m. | Ballroom F |

**Thursday, July 11**

| | | |
|---|---|---|
| Registration | 7:30 a.m. to 11:30 a.m. | Ballroom Pre-function Area |
| Session: ICME Challenges and Education | 8:00 a.m. to 11:35 a.m. | Ballroom D&E |
| Short Course Registration | Noon to 2:00 p.m. | Ballroom Pre-function Area |
| Introduction to Computational Materials Science and Engineering Tools Short Course | 1:00 p.m. to 8:30 p.m. | Salon H |

**Friday, July 12**

| | | |
|---|---|---|
| Continuation of Introduction to Computational Materials Science and Engineering Tools Short Course | 8:30 a.m. to 6:00 p.m. | Salon H |

## TABLE OF CONTENTS

# Welcome to

TMS ICME
MANUFACTURING
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MATERIALS

# 2nd World Congress
## on Integrated Computational Materials Engineering (ICME)

**July 7-11, 2013**
**Salt Lake Marriott Downtown at City Creek**
**Salt Lake City, Utah, USA**

On behalf of The Minerals, Metals & Materials Society (TMS) and the congress organizers, we are pleased to welcome you to this premier event. The Materials Science and Engineering field is at a critical point in its evolution, in large part due to our community's bold vision for the future materials discovery, development, manufacture, and deployment through the Materials Genome Initiative and Integrated Computational Materials Engineering (ICME). Building on the great success of the 1st World Congress on Integrated Computational Materials Engineering in 2011, the 2nd World Congress on ICME (ICME 2013) will convene ICME stakeholders – including researchers, educators, and engineers – to discover the recent global advancement of ICME as an engineering discipline. The final report of a TMS-led study on ICME Implementation in the Automotive, Aerospace, and Maritime Industries will also be released at ICME 2013.

We look forward to an exciting meeting of dynamic discussions, outstanding speakers and interactive poster sessions, and we thank you for your participation in ICME 2013!

Warmest regards on behalf of the ICME 2013 Organizing Committee.

# ABOUT THE CONGRESS

## REGISTRATION

Your full congress registration includes one copy of the proceedings. Your badge ensures admission to each of these events:

- Technical and Poster Sessions
- Access to the Exhibition
- Sunday Welcome Reception
- Monday and Tuesday Poster Receptions
- Wednesday Congress Dinner

### REGISTRATION HOURS

The registration desk will be located in the Ballroom Pre-function Area.

**Sunday**
6:00 p.m. to 9:00 p.m.

**Monday**
7:30 a.m. to 4:30 p.m.
7:30 p.m. to 8:30 p.m.

**Tuesday**
7:30 a.m. to 4:30 p.m.
7:30 p.m. to 8:30 p.m.

**Wednesday**
7:30 a.m. to 5:30 p.m.

**Thursday**
7:30 a.m. to 11:30 a.m.

Short course registration will be open from noon to 2:00 p.m. on Thursday in the Ballroom Pre-function Area.

### INTERNET ACCESS

Complimentary internet access is available for ICME attendees in public areas of the hotel and in the guest rooms.


### TECHNICAL SESSIONS

All oral presentations will be held in Ballrooms D&E of the Marriott Downtown at City Creek. All poster presentations will be held in Ballroom AB&C. See the Technical Program on pages 11-18 for room locations.

### PROCEEDINGS

Full congress registrants receive one copy of the proceedings as part of the registration fee. Additional copies may be purchased for $135 at **www.wiley.com** (TMS members receive a 25% discount). Approximately six weeks after the meeting, individual papers will be available through the Wiley Online Library: **http://onlinelibrary.wiley.com.**

## EXHIBITION

### EXHIBITION HOURS

The exhibition will be located in Ballroom AB&C.

**Monday**
**Set-up:** 9:00 a.m. to noon
2:00 p.m. to 3:30 p.m.
8:00 p.m. to 10:00 p.m.

**Tuesday**
9:00 a.m. to 10:30 a.m.
3:00 p.m. to 4:30 p.m.
8:00 p.m. to 10:00 p.m.

**Wednesday**
8:30 a.m. to 11:30 a.m.
3:30 p.m. to 5:00 p.m.
**Dismantle:** 5:00 p.m. to 8:00 p.m.

TMS would like to thank the Exhibitors and Sponsors on the following pages for their gracious support of the event.

## PLATINUM SPONSOR

### ESI Group Booth #1

ESI Group is a pioneer and world-leading provider in Virtual Prototyping software that takes into account the physics of materials.

ESI Group Virtual Product Engineering allows the manufacturing industry to face the greatest industrial challenge head-on: to deliver innovative products at lower cost, faster and with increased reliability.

ESI aims to give customers across many industry sectors the ability to virtually manufacture and assemble, part by part, complete and physically realistic virtual products that can be tested under normal and exceptional operating conditions. ESI customers can better understand issues related to manufacturing, assembly and coupling between different product attributes and performance domain long before physical prototypes are built and tested.

Virtual Product Engineering enables ESI's customers to get their product cycle right, for the right cost and at the right time. For more info please visit our web-site at: www.esi-group.com

## SILVER SPONSOR

### UES, Inc. Booth #2

RoboMet.3D® is a fully automated, serial sectioning system that generates two-dimensional data for three-dimensional reconstruction. With sectioning rates up to 100 times faster than manual sectioning, Robo-Met.3D collects data in a matter of hours, not months. Robo-Met.3D enables more time for data analysis and characterization and ensures repeatable and accurate data is collected in an efficient and cost-effective manner.

UES, Inc. is an innovative science and technology company that provides its industry and government customers with superior research and development expertise. We create products and services from our technology breakthroughs and successfully commercialize them. UES, Inc. is proud to sponsor ICME for a second year.

## EXHIBITORS

### EDAX Inc. Booth #4

EDAX is a leading provider of innovative materials characterization systems encompassing Energy Dispersive Spectrometry (EDS), Wavelength Dispersive Spectrometry (WDS), Electron Backscatter Diffraction (EBSD) and Micro X-ray Fluorescence (XRF).

EDAX products include standalone tools for EDS, EBSD and WDS, integrated tools for EDS/EBSD, EDS/WDS, and EDS/EBSD/WDS, and a free-standing micro-XRF benchtop elemental analyzer providing small and micro-spot x-ray analysis and mapping.

EDAX develops the best solutions for micro- and nano-characterization, where elemental and/or structural information is required, making analysis easier and more accurate.

EDAX designs, manufactures, distributes and services products for a broad range of industries, educational institutions and research organizations.

### Simpleware Booth #5

Simpleware develops world-leading mesh generation software which converts 3D scan data (e.g. MRI, CT, MicroCT, etc.) into high-quality computer models used for CAD, Finite Element simulation, and Rapid Prototyping. Our Software is being used by engineers in a variety of research fields, including: Biomechanics, Materials Research, Industrial Reverse Engineering, Paleontology, Forensics, and Biomimicry. Simpleware is easy to use and produces more accurate models in a fraction of the time taken with alternative software.

## Thermo-Calc Software Booth #3

Thermo-Calc Software is a leading developer of software and databases for calculations involving computational thermodynamics and diffusion controlled simulations. Thermo-Calc is a powerful tool for performing thermodynamic calculations for multicomponent systems. Calculations are based on thermodynamic databases produced by expert evaluation of experimental data. Databases are available for Al, Mg, steels, Ni-superalloys, Ti, solders and other materials. Programming interfaces are available which enable Thermo-Calc to be called directly from in-house developed software or MatLab. DICTRA is used for accurate simulations of diffusion in multicomponent alloys. TC-PRISMA is a new software package for the simulation of precipitation kinetics in multicomponent alloys.

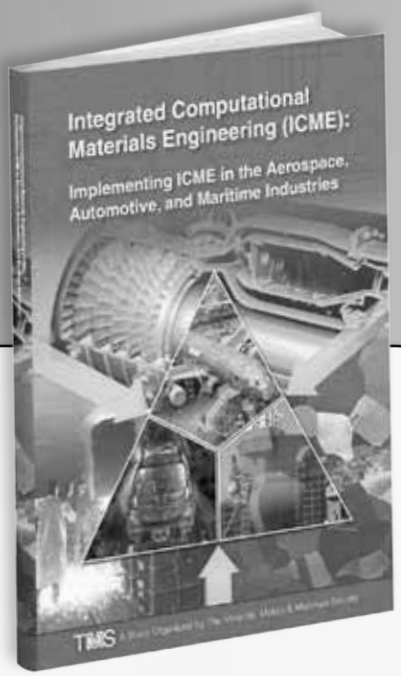
## TMS ICME Implementation Study Booth #6

Learn more about how the TMS-led study on ICME Implementation in the Automotive, Aerospace, and Maritime industries can help you and your organization.

Stop by the TMS booth during breaks to engage with TMS technical staff who will be available to answer your questions about the newly released TMS study.

While you are there, learn how to advocate for ICME in your organization and industry, and explore the many professional development and volunteer opportunities that TMS offers!

# Looking for Ways to Accelerate the Development of New Materials?




Find answers in the latest TMS-produced report:

***Integrated Computational Materials Engineering (ICME): Implementing ICME in the Aerospace, Automotive, and Maritime Industries***

The final report of the TMS-led study* is making its debut at ICME 2013, with each attendee receiving a copy as part of the registration packet. The report is the result of a 14-month study to identify, prioritize, and recommend key steps for rapid implementation of integrated computational materials engineering (ICME) in the automotive, aerospace/aircraft, and maritime industries.

The ICME discipline uses predictive computational tools combined with critical experiments to accelerate and significantly reduce costs associated with the design and manufacturing of new materials systems. ICME is suitable for a variety of industries, providing benefits across the engineering and product development cycle.

## Report Highlights

- Current state of ICME
- Frameworks and toolsets for incorporating ICME into accelerated product development programs in aerospace, automotive and maritime industries
- Identification of crosscutting ICME implementation issues across industrial sectors
- Creating the business case for ICME
- Near-term opportunities for rapid ICME implementation
- Recommendations for overcoming barriers to implementation
- Workforce development for the next generation of ICME integrators
- And more!

## Who Should Read the Report?

The report is useful for a broad variety of stakeholders within and beyond the materials community:

- Professionals and leaders in the aerospace, automotive and maritime industries
- Professionals in other materials-intensive industries
- University professors, researchers, students, and higher-level managers
- Government scientists and engineers, program officers, and policy makers

* Sponsored by the U.S. Department of Defense, the U.S. Department of Energy, and the National Science Foundation, this project also strongly supports the U.S. Materials Genome Initiative (MGI) goals to accelerate the discovery and deployment of new products and increase global competitiveness.

TMS

Download the full report at: **www.tms.org/ICMEstudy**

# POLICIES

## BADGES

All attendees must wear registration badges at all times during the congress to ensure admission to events included in the paid fee such as technical sessions, exhibition and receptions.

## REFUNDS

The deadline for all refunds was June 14, 2013. No refunds will be issued at the congress. Fees and tickets are nonrefundable.

## PHOTOGRAPHY NOTICE

By registering for this congress, all attendees acknowledge that they may be photographed by congress personnel while at events and that those photos may be used for promotional purposes.

## AUDIO/VIDEO RECORDING POLICY

Recording of sessions (audio, video, still photography, etc.) intended for personal use, distribution, publication, or copyright without the express written consent of TMS and the individual authors is strictly prohibited.

## AMERICANS WITH DISABILITIES ACT

The federal Americans with Disabilities Act (ADA) prohibits discrimination against, and promotes public accessibility for, those with disabilities. In support of, and in compliance with ADA, we ask those requiring specific equipment or services to contact TMS Meeting Services at mtgserv@tms.org in advance.

## CELL PHONE USE

In consideration of attendees and presenters, we kindly request that you minimize disturbances by setting all cell phones and other devices on "silent" while in meeting rooms.

## RECYCLING

At the end of the meeting, discard badges and programs in the bins located in the Registration area.

# NETWORKING & SOCIAL EVENTS

## WELCOME RECEPTION

The Welcome Reception will be held on Sunday, July 7 from 10:00 p.m. to midnight in Ballroom F.

## POSTER VIEWING AND RECEPTION

Poster viewing and reception are planned for Monday and Tuesday from 8:00 p.m. to 10:00 p.m. following the technical sessions in Ballrooms AB&C. Don't miss this great networking opportunity!

## CONGRESS DINNER

The dinner will be held on Wednesday, July 10 from 8:00 p.m. to 10:00 p.m. in Ballroom F.


Attend the **Introduction to Computational Materials Science and Engineering Tools short course** following this congress!

**July 11-12, 2013**
Salt Lake Marriott Downtown at City Creek
Salt Lake City, Utah, USA

For more information on the workshop, visit the Registration Desk or the Short Course page of the ICME 2013 website at **www.tms.org/ICME2013**.

The 2nd International Congress on

# 3DMS

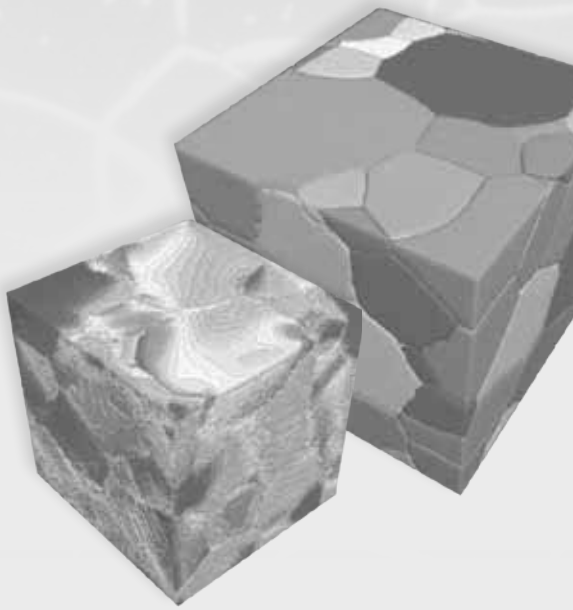
## 3D Materials Science 2014

L'Imperial Palace • Annecy, France • June 29-July 2

## CALL FOR PAPERS

The 3DMS congress series seeks to provide the premier forum for presentations of current interest and significance to the three-dimensional characterization, visualization, quantitative analysis, modeling, and investigation of structure-property relationships of materials. Offering an intimate environment for rich discussions and interactions among key global researchers, 3DMS offers the opportunity to not only assess the state-of-the-art within the various elements of 3D materials science, but to roadmap key areas of future research as well.

The first international 3DMS congress was held in Seven Springs, Pennsylvania, in 2012.



### Submit an Abstract for 3DMS 2014

The 3DMS 2014 technical program will include plenary, keynote and invited lectures, and contributed presentations covering a range of topics representing the most critical and rapidly growing areas of 3D materials science. Abstracts will be accepted on the following topics:

- Experimental techniques for 3D data acquisition
- Advances in reconstruction algorithms
- Image processing and digital representation of 2D and 3D microstructural data
- Advances in 3D materials modeling
- Microstructure property relationships in 3D
- 3D interfaces and microstructural evolution
- Future directions & challenges for 3D materials science

Submit an abstract at **www.tms.org/3DMS2014**

**Abstract Deadline: November 15, 2013**

**Learn more at: www.tms.org/3DMS2014**

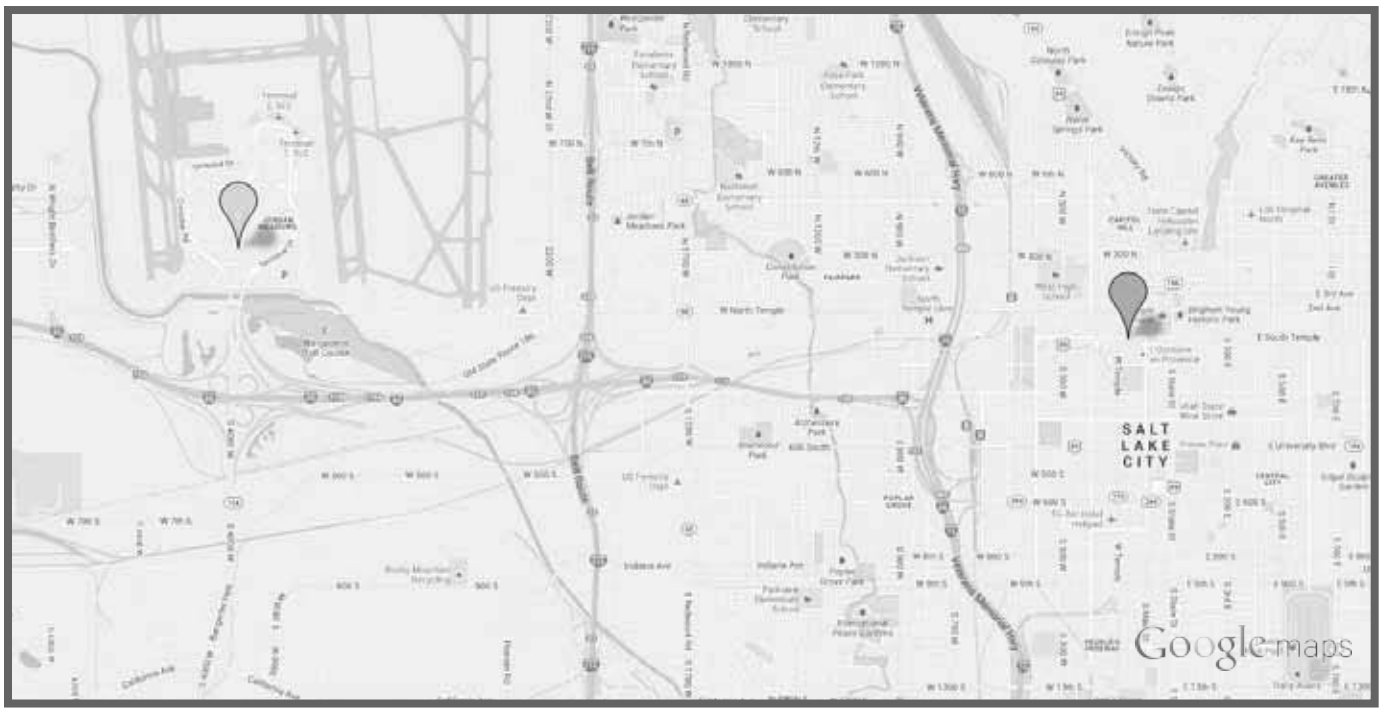
## ABOUT THE VENUE

The Salt Lake Marriott Downtown at City Creek is in the heart of downtown Salt Lake City convenient to shopping, dining, and entertainment, and just 15 minutes from the airport. Guests will appreciate the ideal location adjacent to the unique shopping environment of City Creek Center.

For more information, visit the Housing & Travel page of the ICME website at **www.tms.org/ICME2013**.

The hotel does not provide shuttle service, but the following alternate forms of transportation are available:

- Xpress Shuttle (801-596-1600 or 800-397-0773); fee: $8 USD (one way); reservation required
- Bus service, fee: $2 USD (one way)
- Estimated taxi fare: $25 USD (one way)




: Salt Lake City Airport : Salt Lake Marriott Downtown at City Creek

## SUNDAY, JULY 7, 2013

| Opening Session • Room: Ballroom D&E | |
|---|---|
| 8:00 PM | **Introductory Comments:** Mei Li, Ford Motor Company |
| 8:10 PM | **Invited**<br>**The Importance of Materials and the Opportunity for ICME and MGI: Progress and the Future**: Gerould Young[1]; [1]The Boeing Company |
| 9:00 PM | **The MGI After Two Years:** James Warren[1]; [1]NIST |
| 9:20 PM | **Implementing ICME in the Automotive, Aerospace, and Maritime Industries: Results of a TMS-led Study on ICME Implementation:** George Spanos[1]; David Howe[1]; [1]TMS |

## MONDAY, JULY 8, 2013

| ICME Success Stories and Applications • Room: Ballroom D&E | |
|---|---|
| 8:00 AM | **Introductory Comments:** Elizabeth Holm, Carnegie Mellon University |
| 8:05 AM | **Invited**<br>**Validating ICME Models Across the Length Scales using 4D Synchrotron Imaging:** Peter D. Lee[1]; Chedtha Puncreobutr[1]; Biao Cai[1]; Shyamprasad Karagadde[1]; Lang Yuan[2]; [1]The University of Manchester; [2]GE Global Research |
| 8:35 AM | **Invited**<br>**Microstructural Design for Higher Strength Al Alloys:** Hong Liu[1]; Yipeng Gao[2]; Yunzhi Wang[2]; Jian-Feng Nie[1]; [1]Monash University; [2]The Ohio State University |
| 9:05 AM | **Question and Answer Period** |
| 9:15 AM | **ICME Successes: From Genome to Flight:** Greg Olson[1]; [1]Northwestern University |
| 9:35 AM | **Predicting Fatigue Crack Initiation in Turbine Disk Alloys**: Tresa Pollock[1]; Jean-Charles Stinville[1]; McLean Echlin[1]; [1]University of California Santa Barbara |
| 9:55 AM | **Break** |
| **ICME Applications: Lightweight Materials • Room: Ballroom D** | |
| 10:15 AM | **Application of Computational Thermodynamics and CALPHAD in Magnesium Alloy Development:** Alan Luo[1]; [1]General Motors Global Research and Development |
| 10:35 AM | **ICME Modeling of a Super Vacuum Die Cast (SVDC) AZ91 Magnesium Automotive Component:** Mei Li[1]; Junsheng Wang[1]; Jiashi Miao[2]; Bita Ghaffari[1]; Long-Qing Chen[3]; John Allison[2]; [1]Ford Motor Company; [2]University of Michigan; [3]Penn State University |
| 10:55 AM | **Modelling Precipitation Kinetics during Aging of Al-Mg-Si Alloys:** Qiang Du[1]; Jesper Friis[1]; [1]SINTEF |
| 11:15 AM | **Modeling Processing-Property Relationships to Predict Final Aluminum Coil Quality:** Kai Karhausen[1]; Stefan Neumann[1]; Galyna Laptyeva[1]; [1]Hydro Aluminium Rolled Products GmbH |
| **ICME Applications: Composites • Room: Ballroom E** | |
| 10:15 AM | **Novel Braided and Woven Metallic Structures:** Richard Fonda[1]; Kevin Hemker[2]; Keith Sharp[3]; James Guest[2]; Andrew Geltmacher[1]; Timothy Weihs[2]; David Dunand[4]; Peter Voorhees[4]; Arthur Heuer[5]; [1]Naval Research Laboratory; [2]Johns Hopkins University; [3]3TEX Inc; [4]Northwestern University; [5]Case Western Reserve University |
| 10:35 AM | **CANCELLED: Sequential Approximate Optimization Based Robust Design of SiC-$Si_3N_4$ Nanocomposite Microstructures:** Vikas Tomar[1]; [1]Purdue University |
| 10:55 AM | **Integrating the Influence of Manufacturing Processes in the Design of Composite Components:** Adi Sholapurwalla[1]; Mathilde Chabin[1]; [1]ESI Group |
| 11:15 AM | **Simulation of Curing Process and Prediction of Material Properties for Thermosetting Polymers and Polymer-based Composites:** Chunyu Li[1]; Alejandro Strachan[1]; [1]Purdue University |
| **ICME Applications: Non-Ferrous • Room: Ballroom D** | |
| 1:35 PM | **Casting Simulation of an Aero Engine Structural Component to Characterize the Effect of Alloy Composition:** Benjamin Peterson[1]; Michael Vinup[1]; [1]Honeywell Aerospace |
| 1:55 PM | **Process Simulation Role in the Development of Metal Casting Processes Based on an Integrated Computational Materials Engineering Approach:** Adrian Sabau[1]; Wallace Porter[1]; Hebi Yin[1]; [1]Oak Ridge National Laboratory |

| | |
|---|---|
| 2:15 PM | **Incorporation of Residual Stresses into Design of Ni-Base Superalloy Structures: A Foundational Engineering Problem in Integrated Computational Materials Engineering (ICME):** Michael Caton[1]; [1]US Air Force Research Laboratory |
| 2:35 PM | **Break** |
| 2:55 PM | **Residual Stress Modeling in Aluminum Wrought Alloys:** Bowang Xiao[1]; Qigui Wang[1]; Cherng-Chi Chang[1]; Josie Rewald[1]; [1]GM Powertrain |
| 3:15 PM | **Finite Element Study of the Aluminum AA6111T4 Blanking Process and Its Influence on Sheet Stretchability:** Xiaohua Hu[1]; Dong Mhung Suh[1]; Kyoo Sil Choi[1]; Xin Sun[1]; Sergey Golovaschenko[2]; [1]Pacific Northwest National Laboratory; [2]Ford Research and Advanced Engineering |
| 3:35 PM | **Effects of Pore Distribution Features on Ductility of Mg Castings:** Kyoo Sil Choi[1]; Xin Sun[1]; Dongsheng Li[1]; Mei Li[2]; John Allison[3]; [1]PNNL; [2]Ford Motor Company; [3]University of Michigan |
| 3:55 PM | **Phase-field Simulations of Grain Growth in a Thermal Gradient:** Tao Jing[1]; Qiwei Zheng[1]; [1]Tsinghua University |
| **ICME Applications: Ferrous • Room: Ballroom E** | |
| 1:35 PM | **An Integrated Computational Approach to Predicting the Transition from Internal to External Oxidation of Advanced Alloys in Extreme Environments:** Zi-Kui Liu[1]; Adri van Duin[1]; John Kitchin[2]; Andrew Gellman[2]; Brian Gleeson[3]; Guofeng Wang[3]; Michael Gao[4]; DeNyago Tafen[4]; Youhai Wen[5]; Dominic Alfonso[5]; Bryan Morreale[5]; David Alman[5]; [1]The Pennsylvania State University; [2]Carnegie Mellon University; [3]The University of Pittsburgh; [4]National Energy Technology Laboratory - URS Corporation; [5]National Energy Technology Laboratory |
| 1:55 PM | **ICME Approach to Corrosion Pit Growth Prediction:** Ken Smith[1]; Lei Chen[1]; Rob Darling[1]; Mark Jaworowski[1]; Susanne Opalka[1]; George Zafiris[1]; Thomas Garosshen[1]; Sonia Tulyani[1]; [1]United Technologies Research Center |
| 2:15 PM | **Multiscale Model for Non-metallic Inclusions/Steel Composite System using Data Science Enabled Structure-Property Linkages:** Akash Gupta[1]; Ahmet Cecen[2]; Sharad Goyal[1]; Amarendra Singh[1]; Surya Kalidindi[3]; [1]TRDDC-TCS Innovation Labs, Tata Consultancy Services Ltd.; [2]Department of Mechanical Engineering and Mechanics, Drexel University; [3]Woodruff School of Mechanical Engineering, Georgia Institute of Technology |
| 2:35 PM | **Break** |
| 2:55 PM | **Steel - Ab initio: Quantum Mechanics Guided Design of New Fe Based Materials:** Ulrich Prahl[1]; Wolfgang Bleck[1]; Alireza Saeed-Akbari[1]; [1]RWTH Aachen University |
| 3:15 PM | **An Integrated Model for Microstructure Development in the Heat Affected Zone of an X80 Linepipe Steel:** Warren Poole[1]; M. Militzer[1]; T. Garcin[1]; [1]The University of British Columbia |
| 3:35 PM | **ICME Implementation for Steel Ingot Manufacturing & Conversion:** Patrick Anderson[1]; Stephanie Will[1]; E. Buddy Damm[1]; [1]The Timken Company |
| 3:55 PM | **CANCELLED: Finite Element Modeling of Gear Hobbing and Milling:** Troy Marusich[1]; Deyao Ren[1]; Shuji Usui[1]; Jon Wadell[1]; Wenyang Liu[1]; [1]Third Wave Systems |

**Poster Session I: Modeling, Data and Infrastructure Tools • Room: Ballroom AB&C**

**PI-1: 3D X-ray Diffraction Contrast Tomography Reconstruction of Polycrystalline Strontium Titanate during Sintering and EBSD Validation**: Peter Gumbsch[1]; B. Loedermann[2]; A. Graff[1]; A. Trenkle[2]; M. Syha[2]; D. Weygand[2]; W. Ludwig[3]; [1]Fraunhofer IWM; [2]Institute for Applied Materials IAM; [3]European Synchrotron Radiation Facility

**PI-2: A Brief Review of Precipitation Hardening Models for Aluminum Alloys**: Guannan Guo[1]; Qigui Wang[2]; Gang Wang[3]; Yiming Rong[1]; [1]Worcester Polytechnic Institute; [2]GM-Global Powertrain Engineering; [3]Tsinghua University

**PI-3: A Computational Method for Activation Energy Calculation using Non-isothermal Conditions, Linear Heating Rate and Cubic Spline Interpolation Technique**: Rabindranath Ray[1]; [1]NIT DURGAPUR

**PI-4: A Cross-slip Mechanism of Intermittent Plasticity in Nano- and Micro-pillars**: Tamer Crosby[1]; Nasr Ghoniem[1]; [1]UCLA

**PI-5: A Machine Learning Framework for Efficient EBSD Microscopy Applied to AZ31**: Travis Rampton[1]; David Fullwood[1]; [1]Brigham Young University

**PI-6: A Multi-scale Model to Simulate Forming Limit Diagram of Aluminum Sheets**: Kaan Inal[1]; Abhijit Brahme[1]; Raja Mishra[2]; [1]University of Waterloo; [2]General Motors Research and Development

**PI-7: A Three-dimensional Lattice Boltzmann Model for Columnar Dendrite Growth**: Mohsen Eshraghi[1]; Bohumir Jelinek[1]; Sergio Felicelli[1]; [1]Mississippi State University

**PI-8: Building 3D Microstructure Database using an Advanced Metallographic Serial Sectioning Technique and Robust 3D Segmentation Tools**: Umesh Adiga[1]; Murali Gorantla[1]; James Scott[1]; Daniel Banks[1]; Yoon-Suk Choi[1]; [1]UES, Inc

**PI-9: CALPHAD File Repositories: Increasing Efficiency and Reproducibility**: Carelyn Campbell[1]; Ursula Kattner[1]; Laura Bartolo[2]; [1]National Institute of Standards and Technology; [2]Kent State University

**PI-10: Coupled Composition-Microstructure Modeling of a U-Pu-Zr Fuel**: Jordan Cox[1]; Eric Homer[1]; Veena Tikare[2]; [1]Brigham Young University; [2]Sandia National Laboratories

**PI-11: Creating an Integrated, Community-Sourced, First-Principles Data Repository**: Richard Taylor[1]; Benjamin Burton[1]; Laura Bartolo[2]; [1]NIST; [2]Kent State University

**PI-12: Crystal Plasticity Finite Element Modeling of Single Crystal Niobium Tensile Tests with Weighted Dynamic Hardening Rule**: Aboozar Mapar[1]; Thomas Bieler[1]; Farhang Pourboghrat[1]; Christopher Compton[2]; [1]Michigan State University; [2]Michigan State Univerity

**PI-13: Data Science Enabled Structure Property Correlation for Dual Phase Steel**: Prabhash Kumar[1]; Akash Gupta[1]; Sharad Goyal[1]; Amarendra Singh[1]; Surya Kalidindi[2]; [1]TRDDC, Tata Consultancy Services; [2]Georgia Institute of Technology

**PI-14: Determination of the Characteristic Sizes of Complex Microstructures and Its Application to the Design of Composite Materials**: Victor Chan[1]; James Dempsey[1]; Katsuyo Thornton[1]; [1]University of Michigan, Ann Arbor

**PI-15: Dislocation Density Based Crystal Plasticity Finite Element Model of Polycrystals with Grain Boundary Effect**: Zhe Leng[1]; Alankar Alankar[2]; David Field[1]; Nathalie Allain-Bonasso[3]; Francis Wagner[3]; [1]Washington State University; [2]Los Alamos National Laboratory; [3]University of Metz

**PI-16: Effect of Primary $Al_3Sc$ Particles on Fatigue Behavior Studied through Experimentation and Simulation**: Nilesh Kumar[1]; Mageshwari Komarasamy[1]; Rajiv Mishra[1]; [1]University of North Texas

**PI-17: Establishing the Ni-Fe-Cr-Al-O Thermodynamic Database: DFT Calculations, CALPHAD Modeling and Experiments**: Bi-Cheng Zhou[1]; Michael Gao[2]; ShunLi Shang[1]; Cuiping Guo[1]; Ömer Dogan[3]; Zi-Kui Liu[1]; [1]The Pennsylvania State University; [2]National Energy Technology Laboratory; [3]URS Corporation

**PI-18: Fracture Mode of a Ni-based Single Crystal Superalloy Containing Topologically-Close-Packed Phases at Ambient Temperature**: Qianying Shi[1]; Xianfei Ding[1]; Yunrong Zheng[1]; Jingyang Chen[1]; Qiang Feng[1]; [1]University of Science and Technology Beijing

**PI-19: Interaction of Point Defects with Twin Boundaries in Au: A Molecular Dynamics Approach**: Babar Khan[1]; [1]Central China Normal University

**PI-20: Investigation of γ' Precipitation in Ni-base Superalloy PWA1480 by Interrupted Cooling Coupled with Thermo-kinetic Simulation**: Erwin Povoden-Karadeniz[1]; Markus Kozeschnik[2]; Ernst Kozeschnik[3]; [1]Vienna University of Technology; [2]Graz University of Technology; [3]Vienna University of Technology, Institute of Materials Science and Technology

**PI-21: CANCELLED: Micromechanical Stereoinference**: Thomas Hardin[1]; Brent Adams[1]; Eric Homer[1]; David Fullwood[1]; [1]Brigham Young University

**PI-22: Multi-physics, Multi-scale Simulations of MEMS with Quantified Uncertainties**: Alejandro Strachan[1]; [1]Purdue University

**PI-23: Multiscale Computational Modeling of Adsorption**: Adam Donato[1]; Ranga Pitchumani[1]; [1]Virginia Tech

**PI-24: CANCELLED: Numerical Simulation of Sintering in the Ceramic Oxide**: Mohammed Kadhim[1]; Adill Alwan[2]; Elham Ibraheem[2]; [1]University of Technology; [2]University of Babylon, Babylon, Iraq

**PI-25: Phase Field Modeling of Metal Oxidation Behavior**: Tianle Cheng[1]; Youhai Wen[2]; [1]ORISE; [2]National Energy Technology Laboratory

**PI-26: Phase Formation and Kinetics during Aluminization of Nickel and Nickel-Chromium Wires**: Thomas Philippe[1]; Peter Voorhees[1]; Dinc Erdeniz[1]; David Dunand[1]; [1]Northwestern Universit

**PI-27: Precipitation Simulation of AZ91 Magnesium Alloys**: Chuan Zhang[1]; Weisheng Cao[1]; Shuanglin Chen[1]; Jun Zhu[1]; Fan Zhang[1]; [1]CompuTherm LLC

**PI-28: Reducing the Microstructure Design Space of 2nd Order Homogenization Techniques Using Discrete Fourier Transforms**: Tim Ruggles[1]; Travis Rampton[1]; Scott Rose[1]; David Fullwood[1]; [1]Brigham Young University

**PI-29: Research on Numerical Simulation of the Temperature Field of the Innovation Cathode Cells**: Jiang YanLi[1]; Yu Liang[1]; Feng Naixiang[2]; [1]College of Materials Science and Engineering, Guilin University of Technology; [2]School of Materials & Metallurgy, Northeastern University

**PI-30: Screw Dislocations Cores in Bcc Transition Metals: The Influence of Alloying and Temperature**: Lorenz Romaner[1]; Hong Li[2]; Claudia Ambrosch-Draxl[2]; Reinhard Pippan[3]; [1]Materials Center Leoben; [2]Humboldt-Universität zu Berlin; [3]Erich Schmid Institute

**PI-31: The Simulation as Prediction Tool to Determine the Method of Riser Calculation More Efficient**: Lazaro Suarez[1]; Norge Coello[1]; Alexis Alonso[1]; [1]UCLV

**PI-32: Towards the Interface Level Understanding of Internally Oxidized Metal-oxide Composite Cu-$Al_2O_3$**: Yong Jiang[1]; Guoqiang Lan[1]; Canhui Xu[1]; [1]Central South University

**PI-33: Understanding and Predicting Fatigue Crack Growth from Physical Principles**: Peter Huffman[1]; Scott Beckman[1]; [1]Iowa State University

**PI-34: Using of Automation in Generation of Engineering and Shop Drawings, and 3D Modeling in EPC Projects**: Ali Soheilifar[1]; Erfan Alavi[1]; [1]Sazeh Consultants

## TUESDAY, JULY 9, 2013

**Process Optimization • Room: Ballroom D**

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| 8:20 AM | **Multi-scale, Multi-physics Optimization Framework for Additively Manufactured Structural Components:** Tahany El-Wardany[1]; Mathew Lynch[1]; Wenjiong Gu[1]; Arthur Hsu[1]; Michael Klecka[1]; Aaron Nardi[1]; Daniel Viens[1]; [1]United Technologies Research Center |
| 8:40 AM | **Optimal Process Control through Feature-Based State Tracking along Process Chains:** Melanie Senn[1]; Norbert Link[1]; Peter Gumbsch[2]; [1]Karlsruhe University of Applied Sciences; [2]Fraunhofer Institute for Mechanics of Materials |
| 9:00 AM | **Leveraging ICME for Industrial Applications: Prospects, Progress & Challenges:** Sanjay Sondhi[1]; John Warren[2]; Shesh Srivatsa[2]; Jason Parolini[3]; [1]GE Global Research; [2]GE Aviation; [3]GE Power & Water |
| 9:20 AM | **Application of ICME Methods for the Development of Rapid Manufacturing Technologies:** Tobias Maiwald-Immer[1]; Thomas Goehler[1]; Andreas Fischersworring-Bunk[1]; Carolin Körner[2]; [1]MTU Aero Engines GmbH; [2]University Erlangen-Nürnberg |

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| 9:40 AM | **Break** |
| 10:00 AM | **Introduction of Materials Modelling into Processing Simulation:** Zhanli Guo[1]; Gary Huang[2]; Richard Turner[3]; Alisson da Silva[4]; Nigel Saunders[1]; Hendrik Schafstall[2]; Jean-Philippe Schille[1]; [1]Sente Software Ltd.; [2]Simufact Engineering GmbH; [3]University of Birmingham; [4]Federal University of Minas Gerais |
| 10:20 AM | **An Evolutionary Approach to the Design of Transformation Induced Plasticity (TRIP)-Aided Steels:** Shengyen Li[1]; Raymundo Arroyave[1]; Chung Wang[1]; Ruixian Zhu[1]; Pedro Rivera-Diaz-del-Castillo[2]; Ibrahim Karaman[1]; [1]Texas A&M University; [2]University of Cambridge |
| 10:40 AM | **Analytical Modeling and Performance Prediction of Remanufactured Gearbox Components:** Raja Pulikollu[1]; Nathan Bolander[1]; Sandeep Vijayakar[2]; Matthew Spies[3]; [1]Sentient Science Corporation; [2]Advanced Numerical Solutions LLC; [3]US Army Research Development and Engineering Command |
| 11:00 AM | **A Mechanism-based Hierarchical Model Validated by Experimental Data:** Dongsheng Li[1]; Hussein Zbib[1]; Xin Sun[1]; Mohammad Khaleel[1]; [1]Pacific Northwest National Laboratory |
| **Materials Data for ICME • Room: Ballroom E** | |
| 8:00 AM | **Challenges and Approaches in Materials Data Management for ICME:** Warren Hunt[1]; Ross Brindle[1]; Scott Henry[2]; [1]Nexight Group LLC; [2]ASM International |
| 8:20 AM | **Structuring the Genome: Fundamental Materials Databases:** Greg Olson[1]; [1]Northwestern University |
| 8:40 AM | **Tools to Support the Flow of Traceable Materials Information Needed by ICME:** Will Marsden[1]; Beth Cope[1]; [1]Granta |
| 9:00 AM | **Data Informatics for Phase-Based Property Data:** Carelyn Campbell[1]; Ursula Kattner[1]; Alden Dima[1]; Doug Foxvog[1]; Philippe Dessauw[1]; Pierre Savonitto[1]; [1]National Institute of Standards and Technology |
| 9:20 AM | **Consideration of Ecosystem for Integrated Computational Materials Engineering:** Weiju Ren[1]; [1]Oak Ridge National Laboratory |
| 9:40 AM | **Break** |
| 10:00 AM | **Exploiting Prior Physical Insights via Bayesian Statistics to Develop Accurate Localization Relationships via the Materials Knowledge System:** Tony Fast[1]; [1]University of California Santa Barbara |
| 10:20 AM | **Cross-Scale Cross-Domain Model Validation based on Generalized Hidden Markov Model and Generalized Interval Bayes' Rule:** Yan Wang[1]; David McDowell[1]; Aaron Tallman[1]; [1]Georgia Institute of Technology |
| 10:40 AM | **On the Use of Neural Networks to Develop an Understanding of the Roles of Continuum, Microstructural, and Compositional Variables on the Fracture Toughness of a/ß-processed TIMETAL®6-4:** Peter Collins[1]; Santhosh Koduri[2]; Vikas Dixit[3]; Hamish Fraser[3]; [1]University of North Texas; [2]Intel Corporation; [3]Ohio State University |
| 11:00 AM | **Application of Statistical and Machine Learning Techniques for Correlating Properties to Composition and Manufacturing Process of Steels:** Parijat Deshpande[1]; BP Gautham[1]; Ahmet Cecen[2]; Surya Kalidindi[2]; Ankit Agrawal[3]; Alok Choudhary[3]; [1]Tata Consultancy Services; [2]Drexel University; [3]Northwestern University |
| 11:20 AM | **The GeoDict Virtual Material Laboratory: Integrated Software for Material Analysis and Synthesis:** Andreas Wiegmann[1]; Jürgen Becker[1]; Erik Glatt[1]; Matthias Kabel[2]; Heiko Andrä[2]; [1]Math[2]Market GmbH; [2]Fraunhofer ITWM |
| **Materials Data and Tools • Room: Ballroom D&E** | |
| 2:00 PM | **Introductory Comments:** Peter Gumbsch, Fraunhofer Institute for Mechanics of Materials |
| 2:05 PM | **Invited**<br>**Nanostructuring 1 Billion Tons: Integrating Multiscale Models, High-resolution Characterization and Combinatorial Synthesis for Designing Metallic Alloys:** Dierk Raabe[1]; M. Friak[1]; T. Hickel[1]; J. Millan[1]; S. Sandlöbes[1]; D. Ponge[1]; H. Springer[1]; I. Gutierrez[1]; P. Choi[1]; F. Roters[1]; D. Steinmetz[1]; S. Zaefferer[1]; J. Neugebauer[1]; [1]Max-Planck-Institut |
| 2:35 PM | **Invited**<br>**Microstructure Informatics for Mining Structure-Property-Processing Linkages from Large Datasets:** Surya Kalidindi[1]; [1]Drexel University |
| 3:05 PM | **Invited**<br>**Big Data: A NIST Perspective:** Mary Brady[1]; Alden Dima[1]; [1]National Institute of Standards and Technology |
| 3:35 PM | **Break** |
| 3:45 PM | **Panel Discussion Building a Materials Data Infrastructure for ICME:** Greg Olson, Northwestern University; John Agren, KTH; Matthew J. Zaluzec, Ford; Stephen Christensen, Boeing; James Warren, NIST |
| **Poster Session II: ICME Applications • Room: Ballroom AB&C** | |
| **PII-35: A Computational and Experimental Study of the Vapor Deposition of Thermal Barrier Coatings onto Doublet Turbine Guide Vanes**: Theron Rodgers[1]; Hengbei Zhao[1]; Haydn Wadley[1]; [1]University of Virginia | |
| **PII-36: A Computational Framework for Integrated Process Design for High Performance Parts**: Rajiv Shivpuri[1]; Kuldeep Agarwal[2]; [1]Ohio State University; [2]Minnesota State University | |

**PII-37: A Continuum Model for the Growth of Anodic Alumina Films**: Stephen DeWitt[1]; Katsuyo Thornton[1]; [1]University of Michigan, Ann Arbor

**PII-38: A Large Strain Visoplastic Self-consistent Model with Dynamic Recrystallization Behavior Considered for FCC Polycrystalline Materials at Elevated Temperature**: Xiaohui Fan[1]; Mei Li[2]; Dayong Li[1]; Shaorui Zhang[1]; Yinghong Peng[1]; [1]Shanghai Jiao Tong University; [2]Ford Motor Company

**PII-39: A Microstructure-strength Calculation Model for Predicting Tensile Strength of AlSiMg Alloy Castings**: Shi Yufeng[1]; Liu Baicheng[1]; Xu Qingyan[1]; Wu Qinfang[2]; Yang Hongwei[2]; [1]Tsinghua University; [2]Mingzhi Technology Co., Ltd.

**PII-40: A New Multi-scale Modeling Approach for Characterizing the Mechanical Properties of CNT Composites**: Saeed Herasati[1]; Liangchi Zhang[1]; [1]The University of New South Wales

**PII-41: CANCELLED: An Experimental and Modeling Investigation on High-Rate Formability of Aluminum**: Aashish Rohatgi[1]; Richard Davies[1]; Ayoub Soulami[1]; Elizabeth Stephens[1]; Mark Smith[1]; Gary Vanarsdale[1]; [1]Pacific Northwest National Laboratory

**PII-42: An ICME Approach to Solute Strengthening of Aluminum and Magnesium Alloys**: Louis Hector Jr[1]; Gerard Leyson[2]; William Curtin[3]; David Howe[4]; [1]General Motors; [2]Brown University; [3]Ecole Polytechnique Federal de Lausanne; [4]TMS

**PII-43: An Integrated Approach to Determine Complex Phenomenological Equations in Metallic Systems**: Peter Collins[1]; Iman Ghamarian[1]; [1]University of North Texas

**PII-44: An Integrated Computational and Experimental Study for the Size Effect of the Cu Precipitation on the Mechanical Response of Microalloyed Steel**: Shijin Zhao[1]; Lijuan Hu[1]; [1]Shanghai University

**PII-45: Computational Modeling of Electrochemical Charge/Discharge Behavior of Li-ion Cells**: Madhu Jagannathan[1]; K. S. Ravi Chandran[1]; [1]University of Utah

**PII-46: Design Optimization of Transmission of Si/$SiO_2$ and Ge/$SiO_2$ Multilayer Coatings**: Khurram Iqbal[1]; Jianjun Sha[1]; Asghari Maqsood[2]; [1]Dalian University of Technology; [2]National University of Sciences and Technology

**PII-47: Ductility Prediction for Complex Magnesium Alloy Castings Using Quality Mapping**: Jiang Zheng[1]; Mei Li[1]; Joy Forsmark[1]; Jacob Zindel[1]; John Allison[1]; [1]Ford Motor Company

**PII-48: Electronic, Structural and Elastic Properties of (V,Nb)Cx**: Krista Limmer[1]; Julia Medvedeva[1]; [1]Missouri S&T

**PII-49: Geometric Analysis of Casting Components**: Quan Zhibin[1]; Gao Zhiqiang[1]; Wang Qigui[2]; Sun Yunxia[1]; Chen Xin[1]; Wang Yucong[2]; [1]Southeast University, China; [2]General Motors Holdings LLC

**PII-50: Integrated Computational Materials Education Summer School**: Larry Aagesen[1]; Anton Van der Ven[1]; Jonathan Guyer[2]; Laura Bartolo[3]; Greg Olson[4]; John Allison[1]; Paul Mason[5]; Edwin Garcia[6]; Mark Asta[7]; Katsuyo Thornton[1]; [1]University of Michigan; [2]National Institute of Standards and Technology; [3]Kent State University; [4]Northwestern University; [5]Thermo-Calc Software; [6]Purdue University; [7]University of California Berkeley

**PII-51: Integrated Computational Model for Resistance Spot Welds in Auto-body Crashworthiness CAE: Process, Properties, and Performance**: Lili Zheng[1]; Yanli Wang[1]; Srdjan Simunovic[1]; Wei Zhang[1]; Zhili Feng[1]; [1]Oak Ridge National Laboratory

**PII-52: Integrated Realization of Engineered Materials and Products: A Foundational Problem**: Janet Allen[1]; Farrokh Mistree[1]; Jitesh Panchal[2]; BP Gautham[3]; Amarendra Singh[3]; Sreedhar Reddy[3]; Nagesh Kulkarni[3]; Prabhash Kumar[3]; [1]University of Oklahoma; [2]Purdue University; [3]TRDDC, Tata Consultancy Services

**PII-53: Microstructure Mediated Design of Material and Product**: Ayan Sinha[1]; Janet Allen[2]; Jitesh Panchal[1]; Farrokh Mistree[3]; [1]Purdue University; [2]University of Oklahoma, Norman; [3]University of Oklahoma

**PII-54: Modeling and Verification of Vacuum Carburizing Process for 20$Cr_2Ni_4$A Steel**: Shaopeng Wei[1]; Gang Wang[1]; Yiming Rong[1]; [1]Tsinghua University

**PII-55: Modelling the Process Chain of Cold Rolled Dual Phase Steel for Automotive Application**: Ulrich Prahl[1]; Ali Ramazani[1]; [1]RWTH Aachen University

**PII-56: Multi-Objective Optimization of Wrought Magnesium Alloy Microstructure for Strength and Ductility**: Bala Radhakrishnan[1]; Sarma Gorti[1]; Srdjan Simunovic[1]; [1]Oak Ridge National Laboratory

**PII-57: Multi-Scale Modeling of Ni/YSZ Fuel Cell Anode**: Ji Hoon Kim[1]; Wing Kam Liu[2]; Christopher Lee[2]; [1]Korea Institute of Materials Science; [2]Northwestern University

**PII-58: Quantitative Characterization of Precipitate Microstructures for Use in ICME Models for Magnesium Alloys**: Jiashi Miao[1]; [1]University of Michigan

**PII-59: Study of Numerical Simulation on Quenching Distortion in a Steel Component with Internal Thread**: ZhenGuo Nie[1]; Gang Wang[1]; Yiming (Kevin) Rong[1]; [1]Tsinghua University

**PII-60: The Finite Element Analysis of Thermal Field and Stress Field in the Heavy Locomotive Wheels**: ZhenGuo Nie[1]; Wei Shi[1]; Gang Wang[1]; Yiming (Kevin) Rong[1]; [1]Tsinghua University

**PII-61: The Microstructure and Micromechanical Properties of Zr-Cu-Fe-Al Bulk Metallic Glass Irradiated by High-energy $Ar^+$ Ion**: Bin Yang[1]; Wendong Luo[1]; Lu Yang[2]; Xitao Wang[1]; [1]University of Science and Technology Beijing; [2]Department of Metallurgical Engineering, The University of Utah

**PII-62: The Study on the Induction Heating System: The Establishment of Analytical Model with Experimental Verification and the Phenomenological Study on the Process from Simulation Perspective**: Tianxing Zhu[1]; Feng Li[1]; Xuekun Li[1]; Yiming Rong[2]; [1]Tsinghua University; [2]Worcester Polytechnic Institute

**PII-63: Towards an Integrative Simulation of Microstructural Response to Case Hardening of Microalloyed Steels**: Patrick Fayek[1]; Thomas Petermann[1]; Ulrich Prahl[1]; [1]RWTH Aachen University

**PII-64: Two Thermal Conductivity Analysis of the Fuel Cell Zirconia Electrolyte, Evaluating the Point of Inflection**: Oleksandr Kyrpa[1]; [1]Frantsevich Institute of Problems of Materials Science

**PII-65: Validation of High Strength Cast Al-Zn-Cu-Mg Aluminum for Use in Manufacturing Process Design**: Maria Diana David[1]; Robin Foley[1]; John Griffin[1]; Charles Monroe[1]; [1]University of Alabama at Birmingham

**PII-66: Virtual Prototyping of Lightweight Designs Made with Cold and Hot Formed Tailored Solutions**: Harald Porzner[1]; [1]ESI North America

## WEDNESDAY, JULY 10, 2013

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| **ICME Building Blocks: Opening Session • Room: Ballroom D&E** | |
| 8:00 AM | **Invited**<br>**The Role of First-principles Calculations in ICME Approaches:** Chris Wolverton[1]; [1]Northwestern University |
| 8:30 AM | **Invited**<br>**High-Throughput Experimental Tools for ICME:** Ji-Cheng Zhao[1]; [1]The Ohio State University |
| 9:00 AM | **Question and Answer Period** |
| 9:10 AM | **Break** |
| **ICME Building Blocks: Experimental Tools • Room: Ballroom D** | |
| 9:30 AM | **Experimental Advances for ICME:** Richard Fonda[1]; David Rowenhorst[1]; [1]Naval Research Laboratory |
| 9:50 AM | **Quantitative Characterization of Precipitate Microstructures for Use in ICME Models for Magnesium Alloys:** Jiashi Miao[1]; Emmanuelle Marquis[1]; Mei Li[2]; John Allison[1]; [1]University of Michigan; [2]Ford Research Laboratory |
| 10:10 AM | **Advanced Dilatometry and Calorimetry for the Validation of Materials Mechanical and Transformation Models:** Michael Reich[1]; Benjamin Mikereit[1]; Olaf Kessler[1]; Matthias Krawutschke[1]; Christoph Schick[1]; Jan Kalich[2]; [1]University of Rostock; [2]Dresden University of Technology |
| 10:30 AM | **Non-contact Methods for Determination of Thermodynamic and Thermophysical Properties of High-temperature Materials:** Robert Hyers[1]; Jan Rogers[2]; [1]University of Massachusetts; [2]NASA MSFC |
| 10:50 AM | **Break** |
| 11:10 AM | **3D Image Based Modelling for Computational Materials Applications - Taking 3D Imaging beyond Visualisation:** Philippe Young[1]; Simon Richards[2]; [1]University of Exeter; [2]Simpleware Ltd. |
| 11:30 AM | **The 3D X-ray Crystal Microscope: An Unprecedented Tool for ICME:** Gene Ice[1]; John Budai[1]; Eliot Specht[1]; Bennett Larson[1]; Judly Pang[1]; Rozaliya Barabash[1]; Wenjun Liu[2]; Jonathan Tischler[2]; [1]Oak Ridge National Laboratory; [2]Argonne National Laboratory |
| 11:50 AM | **Model Validation for Microstructural Sensitivities Using High Energy Diffraction Microscopy:** Nathan Barton[1]; Joel Bernier[1]; Moono Rhee[1]; Shui Li[1]; John Bingert[2]; Jonathan Lind[3]; [1]Lawrence Livermore National Laboratory; [2]Los Alamos National Laboratory; [3]Carnegie Mellon University |
| 12:10 PM | **Atom Probe Microscopy:** Anna Ceguerra[1]; Simon Ringer[1]; [1]The University of Sydney |
| **ICME Building Blocks: First Principles and Atomistic Tools • Room: Ballroom E** | |
| 9:30 AM | **Validation of Atomistic Models within an Integrated Computational Environment:** Paul Saxe[1]; Clive Freeman[1]; Erich Wimmer[2]; [1]Materials Design, Inc.; [2]Materials Design, S.A.R.L. |
| 9:50 AM | **What Are the Challenges to Acceptance of Molecular Simulation in Engineering and Design?:** Chandler Becker[1]; Eric Lass[1]; [1]NIST |
| 10:10 AM | **Thermodynamic Properties of Paramagnetic Iron from Non-collinear DFT Calculations:** Vsevolod Razumovskiy[1]; Andrei Ruban[2]; Andrei Reyes-Huamantinco[1]; [1]Materials Center Leoben; [2]KTH Royal Institute of Technology |
| 10:30 AM | **3D Hybrid Atomistic Modeling of ß" in Al–Mg–Si: Putting the Full Coherency of a Needle Shaped Precipitate to the Test:** Flemming Ehlers[1]; Stéphane Dumoulin[2]; Randi Holmestad[1]; [1]Norwegian University of Science and Technology, NTNU; [2]SINTEF, Materials and Chemistry |
| 10:50 AM | **Break** |
| 11:10 AM | **First Principles Computational Determination of Anisotropic Elastic Constants of Hard Compounds (Borides) Through Density Functional Theory:** K. S. Ravi Chandran[1]; K. Panda[1]; [1]University of Utah |
| 11:30 AM | **Ab Initio Determination of Interfacial Energetics of Alloys:** Liang Qi[1]; Maarten de Jong[1]; Mark Asta[1]; [1]University of California, Berkeley |
| 11:50 AM | **Molecular Dynamics and Experimental Characterization of Martensitic Transformations in CoNiAl Alloys:** Vesselin Yamakov[1]; Terryl Wallace[2]; John Newman[2]; Ganga Purja Pun[3]; Yuri Mishin[3]; [1]National Institute of Aerospace; [2]NASA Langley Research Center; [3]George Mason University |

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| 12:10 PM | **Site Preference and Interaction Energies of Co and Cr in Gamma Prime $Ni_3Al$: A First Principles Study:** Jincheng Du[1]; Mrunal Chaudhari[1]; [1]University of North Texas |
| 12:30 PM | **Online Atomistic Polymer Simulations at NanoHUB.org:** Benjamin Haley[1]; Chunyu Li[1]; Nathaniel Wilson[1]; Eugenio Jaramillo[2]; Alejandro Strachan[1]; [1]Purdue University; [2]Texas A&M International University |
| **ICME Building Blocks: Computational Thermodynamics and Kinetics • Room: Ballroom D** | |
| 2:30 PM | **The Role of the CALPHAD Approach in ICME:** Fan Zhang[1]; Weisheng Cao[1]; Shuanglin Chen[1]; Chuan Zhang[1]; Jun Zhu[1]; [1]Compu-Therm, LLC |
| 2:50 PM | **An Open Source Thermodynamic Software and Database Structure as Backbone for Application Software in Materials Science:** Bo Sundman[1]; Ursula Kattner[2]; Mauro Palumbo[3]; Suzana Fries[3]; [1]CEA Saclay; [2]NIST; [3]ICAMS, RUB |
| 3:10 PM | **Assessment of Thermodynamic Data by Physically-based Thermo-kinetic Modeling:** Erwin Povoden-Karadeniz[1]; Peter Lang[2]; Ernst Kozeschnik[3]; [1]Vienna University of Technology, CDLESOP; [2]Materials Center Leoben Forschung GmbH; [3]Vienna University of Technology, Institute of Materials Science and Technology |
| 3:30 PM | **Thermodynamic and Kinetic Simulation and Experimental Results Homogenizing Advanced Alloys:** Paul Jablonski[1]; Jeffrey Hawk[1]; [1]US Department of Energy |
| 3:50 PM | **Optimizing Alloy and Process Design Using Thermodynamic and Properties Databases and a Direct Search Algorithm:** Aimen Gheribi[1]; Eve Belisle[1]; Christopher Bale[1]; Sebastien Le Digabel[1]; Charles Audet[1]; Arthur Pelton[1]; [1]Ecole Polytechnique de Montreal |
| 4:10 PM | **Break** |
| 4:30 PM | **Simulations of Precipitate Microstructure Evolution during Heat Treatments:** Kaisheng Wu[1]; Gustaf Sterner[2]; Qing Chen[2]; Herng-Jeng Jou[3]; Johan Jeppsson[2]; Johan Bratberg[2]; Anders Engstrom[2]; Paul Mason[1]; [1]Thermo-Calc Software Inc; [2]Thermo-Calc Software AB; [3]QuesTek Innovations LLC |
| 4:50 PM | **Development of Gradient Cemented Carbides through ICME Strategy:** Yong Du[1]; Yingbiao Peng[1]; Weibin Zhang[1]; Weimin Chen[1]; Peng Zhou[1]; Wen Xie[2]; Kaiming Cheng[1]; Lijun Zhang[1]; Guanghua Wen[2]; Shequan Wang[2]; [1]State Key Lab of Powder Metallurgy, Central South University; [2]Zhuzhou Cemented Carbide Cutting Tools Limited Company |
| 5:10 PM | **Computational Study of Pearlite Growth in Mixed Diffusion-controlled Regime:** Kumar Ankit[1]; Britta Nestler[1]; [1]Institute of Materials and Processes, Karlsruhe Institue of Technology |
| 5:30 PM | **Phase-field Modeling of Microstructure Evolution in Nuclear Fuels under Elastic-plastic Deformation:** Shenyang Hu[1]; Yulan Li[1]; Xin Sun[1]; [1]Pacific Northwest National Laboratory |
| **ICME Building Blocks: Process and Performance Modeling • Room: Ballroom E** | |
| 2:30 PM | **Microstructure-based Modeling and Experimental Validations of Dislocation and Twinning Plasticity in Metals:** Jaafar El-Awady[1]; [1]Johns Hopkins University |
| 2:50 PM | **A Study for the Constitutive Model of Stainless Steel Subjected to High Strain Rate and Temperature:** Yu Jianchao[1]; Jiang Feng[1]; Rong Yiming[1]; [1]Tsinghua University |
| 3:10 PM | **Full-field Multi-scale Modelling of Sheet Metal Forming Taking the Evolution of Texture and Plastic Anisotropy into Account:** Paul Van Houtte[1]; Jerzy Gawad[2]; Eyckens Philip[1]; Albert Van Bael[1]; Giovanni Samaey[1]; Dirk Roose[1]; [1]KULeuven; [2]AGH University of Science and Technology |
| 3:30 PM | **Integrating Quench Modeling into the ICME Workflow:** Andrew Banka[1]; Jeffrey Franklin[1]; William Newsome[1]; [1]Airflow Sciences Corporation |
| 3:50 PM | **Modeling Crack Propagation in Polycrystalline Alloys using Crystal Plasticity Finite Element Method:** Veera Sundararaghavan[1]; Shang Sun[1]; [1]University of Michigan |
| 4:10 PM | **Break** |
| 4:30 PM | **A Coupled Approach to Weld Pool, Phase and Residual Stress Modelling of Laser Direct Metal Deposition (LDMD) Processes:** Mustafa Megahed[1]; Mushtaq Khan[2]; Juansethi Ibara-Medina[2]; Michael Vogel[2]; Narcisse N'Dri[1]; Andrew Pinkerton[3]; [1]ESI Group; [2]University of Manchester; [3]Lancaster University |
| 4:50 PM | **Process Model for Accelerated Cooling of Hot-rolled Low-carbon Steels:** Matthias Militzer[1]; Vladan Prodanovic[1]; Tao Jia[2]; Thomas Garcin[1]; [1]The University of British Columbia; [2]Northeastern University |
| 5:10 PM | **Prediction of the Uncertainty in the Response of Lightweight Structures Consisting of Solid Foams:** Jörg Hohe[1]; Carla Beckmann[1]; [1]Fraunhofer-Institut für Werkstoffmechanik IWM |

## THURSDAY, JULY 11, 2013

| ICME Challenges and Education • Room: Ballroom D&E | |
|---|---|
| 8:00 AM | **Introductory Comments:** Katsuyo Thornton, University of Michigan |
| 8:05 AM | **Invited**<br>**Enabling Elements of Integrated Computational Materials and Manufacturing Science and Engineering (ICM2SE):** David Furrer[1]; [1]Pratt & Whitney |
| 8:35 AM | **ICME – A Mere Coupling of Models or a Discipline on Its Own?:** Markus Bambach[1]; Georg Schmitz[1]; Ulrich Prahl[1]; [1]RWTH Aachen University |
| 8:55 AM | **Knowledge Assisted Integrated Design of a Component and its Manufacturing Process:** BP Gautham[1]; Nagesh Kulkarni[1]; Danish Khan[1]; Pramod Zagade[1]; Rohith Uppaluri[1]; [1]TRDDC, Tata Consultancy Services |
| 9:15 AM | **Break** |
| 9:35 AM | **Invited**<br>**Integrated Computational Materials Education:** Mark Asta[1]; Katsuyo Thornton[2]; [1]University of California, Berkeley; [2]University of Michigan |
| 10:05 AM | **Integrated Computational Materials Engineering (ICME): Education and Workforce Development:** Mark Horstemeyer[1]; [1]Mississippi State University |
| 10:25 AM | **Break** |
| 10:35 AM | **Panel Discussion:** John Allison, University of Michigan; Julie Christodoulou, ORNL; Tresa Pollock, UCSB; George Spanos, TMS |
| 11:25 AM | **Concluding Comments** |

## Opening Sunday Evening Session

Sunday PM Room: Ballroom D&E
July 7, 2013 Location: Salt Lake Marriott Downtown at City Creek

*Session Chair:* Carelyn Campbell, National Institute of Standards and Technology

**8:00 PM Introductory Comments:** Mei Li, Ford Motor Company

**8:10 PM Invited**
**The Importance of Materials and the Opportunity for ICME and MGI: Progress and the Future**: *Gerould Young*[1]; [1]The Boeing Company

Materials have been and will continue to be critical enablers in Aerospace Products. The complexity of aerospace products requires a great deal of effort (time and money) to characterization a material such that we can design and manufacture an new product. Powerful analysis and simulation techniques such as computational fluid dynamics, finite element methods, and computer simulation have taken prominent roles in our design cycle by reducing and focusing the amount of physical testing we do. These computational tools are now available to the materials and process engineer. There are many challenges to this community; how to use these tools to make decisions and learn faster, how to use this tool set to accelerate material characterization and manufacturing process maturation, how integrate existing tool sets together across scales and disciplines to accelerate our development cycles and finally how to develop the new work force and train the existing work force in use of these new tools. This talk with offer some experience and thoughts on how to address these challenges.

**9:00 PM**
**The MGI After Two Years**: *James Warren*[1]; [1]NIST

In the two years since the Materials Genome Initiative was announced, the conversation on how we do materials science has begun to change, but we still have a number of reckonings before these changes take root. Of particular importance is how we view data in materials science, and, within that framework, how empiricism can be enhanced, not just through the introduction of new models, but by using data-driven experimental methods coupled to machine learning to completely redefine the modalities of materials research.

**9:20 PM**
**Implementing ICME in the Automotive, Aerospace, and Maritime Industries: Results of a TMS-led Study on ICME Implementation**: *George Spanos*[1]; David Howe[1]; [1]TMS

Now that Integrated Computational Materials Engineering (ICME) is recognized as a nascent discipline, the materials, manufacturing, and engineering communities are at a critical juncture. ICME implementation on a much wider scale than occurs presently is needed to accelerate the design and manufacturing of a variety of new materials systems while reducing the costs of such development. In order to define the pathway(s) to more rapid implementation of ICME, a focused study was undertaken by The Minerals, Metals & Materials Society (TMS). To accomplish this, TMS convened more than 40 of the leading experts in ICME to identify, prioritize, and make detailed recommendations of the framework and key steps needed for rapid implementation of (ICME) in three critical industrial sectors - the automotive, aerospace, and maritime. This study also addressed cross-cutting ICME issues that apply to all of these sectors (e.g., data management, tool integration….). The study's final report is aimed at becoming a "field manual" for integrated product development teams, ICME practitioners, and/or other engineering groups who wish to implement ICME in their companies, as well as for other scientists, engineers or industrial professionals who want to learn more about ICME implementation. This study could also provide the nuclei of ideas and personnel from which ICME groups could begin to self assemble. TMS coordinated this study on behalf of the Department of Defense, the Department of Energy, and the National Science Foundation. This presentation will provide an overview of the goals, results, and final report of this study.

## ICME Success Stories and Applications

Monday AM Room: Ballroom D&E
July 8, 2013 Location: Salt Lake Marriott Downtown at City Creek

*Session Chair:* John Allison, University of Michigan

**8:00 AM Introductory Comments:** Elizabeth Holm, Carnegie Mellon University

**8:05 AM Invited**
**Validating ICME Models Across the Length Scales using 4D Synchrotron Imaging**: *Peter D. Lee*[1]; Chedtha Puncreobutr[1]; Biao Cai[1]; Shyamprasad Karagadde[1]; Lang Yuan[2]; [1]The University of Manchester; [2]GE Global Research

Integrated computational materials engineering (ICME) simulations require a wide range of material property and validation data. They work across the scales from the atomistic level to macroscopic component behaviour. In this paper we will demonstrate how in situ, time resolved, synchrotron x-ray tomography can be used to measure the thermo-physical properties required for ICME simulations of automotive and aerospace components. Examples will be given ranging from measurement of flow and mechanical properties. The in situ experiments also give insight into which physical mechanisms dominate material/component failure, and allow the simulations to be more computationally effective by focussing on these mechanisms. In addition to using 4D synchrotron Imaging to inform simulations, methods of validating calculations via quantification of damage growth, semi-solid deformation, and freckle formation will be demonstrated in materials ranging from a light alloy for automotive components to Ni-based superalloys for industrial gas turbines. The results demonstrate that in many cases it is the size distribution of initiating defects, and their potency to initiate failure, that is critical. These phenomena are dependent on both deterministic and stochastic factors, and methods for quantify both for model validation will be discussed.

**8:35 AM Invited**
**Microstructural Design for Higher Strength Al Alloys**: Hong Liu[1]; Yipeng Gao[2]; Yunzhi Wang[2]; *Jian-Feng Nie*[1]; [1]Monash University; [2]The Ohio State University

Aluminium alloys have gained wide applications in the aerospace and automotive industries. Many of these alloys owe their high strength to plate-shaped precipitates that are produced by an age hardening process. Despite the importance of these precipitates at both practical and fundamental levels, their formation mechanisms and their effects on precipitation hardening have not been unambiguously established. This presentation will be focused on our results on the characterization of precipitates in selected aluminium alloys using conventional transmission electron microscopy and high-angle annular dark-field scanning transmission electron microscopy and modelling of precipitation and strengthening using phase field modelling. It will be shown that even the well-known precipitate phases in aluminium alloys exhibit structural features hitherto unreported. The modelling results indicate that further improvement in the strength of existing aluminium alloys might be achieved by increasing the number density and/or aspect ratio of the precipitate plates.

**9:05 AM Question and Answer Period**

**9:15 AM**
**ICME Successes: From Genome to Flight**: *Greg Olson*[1]; [1]Northwestern University

The numerical implementation of established materials science principles in the form of purposeful engineering tools has brought a new level of integration of the science and engineering of materials. Building on a system of fundamental databases now known as the Materials Genome, parametric materials design has integrated materials science, applied mechanics and quantum physics within a systems engineering framework to create a first generation of designer "cyberalloys" that have now entered successful commercial applications, and a new enterprise of commercial materials design services has steadily grown over the past decade. The DARPA-AIM initiative broadened computational materials engineering to address acceleration of the full materials development and qualification cycle, and a new level of science-based AIM modeling accuracy has now been achieved under the ONR/DARPA "D3D" Digital Structure consortium. A surface thermodynamic genome database predicted directly from validated DFT quantum mechanical calculations has generated novel "Quantum Steels" completely eliminating intergranular stress corrosion cracking at the highest strength levels. Integration with the full suite of fundamental databases and models has recently demonstrated the historic milestone of accelerated flight qualification for aircraft landing gear through application of the fully integrated computational design + AIM methodology. Past success defines a clear path forward for major enhancement of materials genomics technology.

**9:35 AM**
**Predicting Fatigue Crack Initiation in Turbine Disk Alloys**: *Tresa Pollock*[1]; Jean-Charles Stinville[1]; McLean Echlin[1]; [1]University of California Santa Barbara

Fatigue is a limiting property for nickel-base alloys for turbine disks that operated in aircraft engines and power generation turbines. Cracks typically do not initiate at extrinsic defects, but at intrinsic features of the microstructure. The nature of the microstructural "neighborhoods" that result in fatigue crack initiation has been studied in detail in 3-D using a new TriBeam femtosecond laser-based tomography approach in both low cycle and high cycle fatigue. In data sets that are up to 0.5mm on edge, the combination of grain size, orientation, twin population as well as the neighboring grain orientations influence fatigue crack initiation. The probability of encountering the critical combination of features in a given volume of material is considered along with implications for modeling of fatigue life.

**9:55 AM Break**

## ICME Applications: Lightweight Materials

Monday AM Room: Ballroom D
July 8, 2013 Location: Salt Lake Marriott Downtown at City Creek

*Session Chair:* Alan Luo, General Motors Research & Development

**10:15 AM**
**Application of Computational Thermodynamics and CALPHAD in Magnesium Alloy Development**: *Alan Luo*[1]; [1]General Motors Global Research and Development

This paper summarizes the development of new cast and wrought magnesium alloys using computational thermodynamics and the CALPHAD (CALculation of PHAse Diagrams) approach coupled with critical experimental validation. The work illustrates the role of calculated phase diagrams, solidification paths and phases in predicting and interpreting the final microstructure of Mg-Al-Ca and Mg-Al-Sn cast alloy systems and Mg-Al-Zn/Mn and Mg-Zn-Nd wrought alloy systems.

**10:35 AM**
**ICME Modeling of a Super Vacuum Die Cast (SVDC) AZ91 Magnesium Automotive Component**: Mei Li[1]; *Junsheng Wang*[1]; Jiashi Miao[2]; Bita Ghaffari[1]; Long-Qing Chen[3]; John Allison[2]; [1]Ford Motor Company; [2]University of Michigan; [3]Penn State University

Magnesium applications for the automotive and aerospace industry have become increasingly important due to light-weight and consequent potential to reduce both fuel consumption and green house effect. In this study, Integrated Computational Materials Engineering (ICME) models have been successfully developed to study the effects of casting and heat treatment process on the microstructures and mechanical property of a super vacuum die cast (SVDC) AZ91 automotive shock tower component. Casting and solution treatment process models were developed based on commercial tools. A hybrid phase field-TEM microstructure model was developed for $Mg_{17}Al_{12}$ precipitation kinetics and coupled with mechanical property model to predict the yield strength during aging. The ICME approach was demonstrated to be a critical virtual tool in evaluating and optimising the design and manufacturing process of magnesium alloy castings.

**10:55 AM**
**Modelling Precipitation Kinetics during Aging of Al-Mg-Si Alloys**: *Qiang Du*[1]; Jesper Friis[1]; [1]SINTEF

A classical Kaufmann-Wagner numerical model is employed to predict the evolution of precipitate size distribution during the aging treatment of Al-Mg-Si alloys. One feature of the model is its fully coupling with CALPHAD database, and with the input of interfacial energy obtained from ab-initio calculation, it is able to capture the morphological change of the precipitates. The simulation results will be compared with the experimental measurements.

**11:15 AM**
**Modeling Processing-Property Relationships to Predict Final Aluminum Coil Quality**: *Kai Karhausen*[1]; Stefan Neumann[1]; Galyna Laptyeva[1]; [1]Hydro Aluminium Rolled Products GmbH

In the definition of the term ICME the integration of multiple length-scale models is the key requisite to obtain information required to design products. While product properties are a measure on a macroscopic length scale, they are controlled by the microstructure on a microscopic or even atomistic length-scale. They are generated on production facilities on a very large scale. In translation of the definition of ICME to the production of rolled Aluminum semi-fabricated products alloys and processing routes must be combined to improve the final customer properties to enable the development of new designs and products. Since the relationships between processing conditions, microstructural evolution and derived properties are highly non-linear, this task can only be achieved by computer aided methods. Critical properties of Aluminum coils and sheet are on the one hand the physical and chemical properties of the metal, such as strength, elongation, anisotropy, formability, corrosion resistance etc.. But on the other hand, geometrical tolerances and surface quality are equally important and often result from metallurgical events during processing. In some cases they can be derived from integrated process and microstructure simulation methods as well. This paper describes the state of the art in through process modeling of Aluminum coils and strip with a view of tracing the microstructural development and deriving property information. Especially new approaches to critical parameters such as coil stability and sheet flatness, resulting from microstructural mechanisms are treated by sample computations of industrial processing chains.

## ICME Applications: Composites

Monday AM Room: Ballroom E
July 8, 2013 Location: Salt Lake Marriott Downtown at City Creek

*Session Chair:* Vikas Tomar, Purdue University

**10:15 AM**

**Novel Braided and Woven Metallic Structures**: *Richard Fonda*[1]; Kevin Hemker[2]; Keith Sharp[3]; James Guest[2]; Andrew Geltmacher[1]; Timothy Weihs[2]; David Dunand[4]; Peter Voorhees[4]; Arthur Heuer[5]; [1]Naval Research Laboratory; [2]Johns Hopkins University; [3]3TEX Inc; [4]Northwestern University; [5]Case Western Reserve University

The fabrication of novel structural materials can be a time-consuming and expensive process. However, the incorporation of integrated computational materials engineering (ICME) methodologies can help constrain the design space variables and streamline the material development process. We have assembled a team to develop advanced textile processing methods for the fabrication of woven or braided structures with high stiffness and permeability. To accomplish this goal, we are using topology optimization to design structures optimized so as to maximize stiffness and permeability. These idealized structures are fabricated using novel 3D weaving or braiding techniques with ductile elemental or alloy wire compositions. The stiffness of the resultant structures is then enhanced through reaction of the component wires and joining techniques to bond neighboring wires within that structure. The resultant structures and experimental characterization of their properties will be correlated with the results of both idealized and image-based modeling.

**10:35 AM CANCELLED**

**Sequential Approximate Optimization Based Robust Design of SiC-$Si_3N_4$ Nanocomposite Microstructures**: *Vikas Tomar*[1]; [1]Purdue University

A simulation-based robust design optimization methodology to predict the most suitable microstructures of SiC-$Si_3N_4$ nanocomposites for desired high temperature deformation energy is presented. The focus is on finding robust microstructures that maximize the deformation energy at two temperatures: 1500°C and 1600°C. Finite element based tensile tests are performed on the SiC-$Si_3N_4$ microstructures to extract their deformation energy, which is considered as the area under the force-displacement curve resulting from corresponding tensile tests. A sequential approximate optimization under uncertainty algorithm is applied to six different test problems. The first four cases obtain optimum microstructures at specific temperatures. In the last two cases, the focus is on obtaining optimal microstructures that will perform well at both temperatures. During optimization, statistical uncertainties inherent to computational microstructural generation are quantified by the mean and the standard deviation of the finite element based response analysis. Thereafter, these statistical properties are introduced in the optimization framework based on a combination of a sequential approximate optimization method and a trust region method to obtain a set of microstructures with targeted high deformation energy. The results show that the SiC volume fraction, the number of $Si_3N_4$ grains, grain size distribution of the $Si_3N_4$ grains, and grain size of the SiC grains have varied effects on the deformation energy at different temperatures. At 1500°C the preferred material is the one with higher $Si_3N_4$ volume fraction. On the other hand the preference is on material with higher SiC volume fraction at 1600°C.

**10:55 AM**

**Integrating the Influence of Manufacturing Processes in the Design of Composite Components**: *Adi Sholapurwalla*[1]; Mathilde Chabin[1]; [1]ESI Group

Composites manufacturing simulation is widely used in the industry to define and optimize the manufacturing strategy and desired process conditions. There is significant evidence to show a link between the effects of the manufacturing process on in-life mechanical performance. This raises questions as to the current best-practices in the aerospace and automotive industry, where certain stringent tolerances and weight criteria have to be met. Manufacturing Process Simulation (MPS) is sparingly utilized in the design cycle. Most of the manufacturing effects cannot be accurately predicted so are accounted for in the design stage through a safety factor. This usually leads to added mass which may dramatically alter the low weight benefits of using composite materials. Implementing MPS in the design cycle before a prototype can be built would lead to a precise understanding of the factor of safety leading to an optimum design. In addition to describing the standard benefits of manufacturing simulation through various case studies, the presentation will also illustrate another application of manufacturing simulation – manufacturing simulation for better design verification. The paper will show the need to account for manufacturing effects in composites design through a series of experimental and numerical examples. For instance, the consequences of the reinforcement deformations will be examined and reorientation during draping and porosity during infusion in a Liquid Composite Molding (LCM) process on the failure and damage behavior in mechanical analysis will be studied.

**11:15 AM**

**Simulation of Curing Process and Prediction of Material Properties for Thermosetting Polymers and Polymer-based Composites**: Chunyu Li[1]; *Alejandro Strachan*[1]; [1]Purdue University

Thermoset polymers have increasingly become the popular matrix of polymer composites because of their higher stiffness, higher creep resistance and higher thermal resistance over thermoplastic polymers. A fundamental understanding of the structural evolution and the relationship between material properties and molecular structures at the atomistic level is necessary. Further understanding of the matrix-fiber interaction at the atomistic level is also of significant importance. In this presentation, we will introduce our efforts in simulating the curing process and predicting material properties of themoset polymers by using molecular dynamics (MD). Recently, we developed a procedure to mimic chemical reactions in the curing process of thermosets. The DREIDING force field with environment-dependent atomic charges obtained self consistently during the dynamics was employed in the simulations. Thermo-mechanical properties of the crosslinked systems are obtained from extensive MD simulations. The results are in good agreement with available experimental data and show that atomistic simulations can capture non-trivial trends in polymer physics including the effect of temperature, thermal history and strain rate in yield and post-yield behavior. We also used molecular dynamics simulations to characterize the in-situ curing process of the resin and the thermo-mechanical response of the graphite-reinforced epoxy composites. Both cohesive yield with strain localization and nano-void formation within the bulk polymer and interface de-bonding between graphite and thermoset were observed, depending on the in-plane orientation of graphite. These two mechanisms lead to different post yield behavior and can provide key insight for the development of predictive models of carbon fiber polymer composites.

## ICME Applications: Non-Ferrous

Monday PM Room: Ballroom D
July 8, 2013 Location: Salt Lake Marriott Downtown at City Creek

*Session Chairs:* Michael Caton, US Air Force Research Laboratory; Xin Sun, Pacific Northwest National Laboratory

**1:35 PM**
**Casting Simulation of an Aero Engine Structural Component to Characterize the Effect of Alloy Composition**: *Benjamin Peterson*[1]; Michael Vinup[1]; [1]Honeywell Aerospace

Cast ATI718Plus® alloy was recently developed for applications that require greater high temperature strength capability than conventional alloy 718 with reduced alloy chemistry cost as compared with other higher temperature capable alternatives. The development of this alloy also targeted adequate castability and weldability performance for investment cast applications such as combustor plenums, turbine cases, turbine frames, and other hot section, aero engine structural components. Honeywell Aerospace is currently implementing this alloy by targeting a key, highly complex, cast structural component that requires higher temperature capability. An ICME tool, solidification modeling, is used to minimize the program risk and alloy implementation time. Multiple simulations of available cast alloy chemistries are performed and compared to identify probable locations for casting defects and which alloy alternative would ideally replace the current alloy. Casting simulation parameters are held constant, except for pour temperature, to generate a comparison based on alloy composition. This analysis includes evaluating high stress regions as potential hot-tear locations and an evaluation of the porosity distribution. An over view of these results efforts will be discussed.

**1:55 PM**
**Process Simulation Role in the Development of Metal Casting Processes Based on an Integrated Computational Materials Engineering Approach**: *Adrian Sabau*[1]; Wallace Porter[1]; Hebi Yin[1]; [1]Oak Ridge National Laboratory

To accelerate the introduction of new materials and components, the development of metal casting processes requires the teaming between different disciplines, as multiphysical phenomena have to be considered simultaneously for the process design and optimization of mechanical properties. The required models as well as their validation status for dealing with physical phenomena that need to be considered for metal casting are reviewed. The measurement of property data and validation data is also highlighted. One vehicle to accelerate the development of new materials is through combined experimental-computational efforts, as underlined in Integrated Computational Materials Engineering framework. Integrated computational/experimental practices are reviewed; strengths and weaknesses are identified with respect to metal casting processes. Specifically, the examples are given for the knowledge base established at Oak Ridge National Laboratory and computer models for predicting casting defects and microstructure distribution in Aluminum and Magnesium alloy components.

**2:15 PM**
**Incorporation of Residual Stresses into Design of Ni-Base Superalloy Structures: A Foundational Engineering Problem in Integrated Computational Materials Engineering (ICME)**: *Michael Caton*[1]; [1]US Air Force Research Laboratory

The Materials and Manufacturing Directorate of the Air Force Research Laboratory is investing in a Foundational Engineering Problem (FEP) aimed at incorporating residual stress into the design of Ni-base superalloy structures. FEPs, as conceived in the 2008 National Materials Advisory Board report entitled *Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security*, consist of an advanced engineering component, a materials system, and a manufacturing process that must be rapidly optimized within a more complex engineering system. FEPs are intended to accelerate the development and application of ICME within the industrial base. The presentation will outline the process of developing this FEP topic through a collaborative exchange between the Air Force and a consortium of aerospace industrial members within the Metals Affordability Initiative. The criteria, upon which the proposal selection was based, will be discussed and a high-level description of this recently-initiated, 5-year program will be provided.

**2:35 PM Break**

**2:55 PM**
**Residual Stress Modeling in Aluminum Wrought Alloys**: Bowang Xiao[1]; *Qigui Wang*[1]; Cherng-Chi Chang[1]; Josie Rewald[1]; [1]GM Powertrain

Aluminum wrought alloys are usually subjected to heat treatment which includes quenching after solution treatment to improve aging responses and mechanical properties. Rapid quenching can lead to high residual stress and severe distortion which significantly affect dimension stability, functionality and particularly performance of the product. Following quenching, a mechanical stretching is usually applied to reduce as-quench residual stress and straighten the products. To model residual stress and distortion during heat treatment and mechanical stretching of aluminum wrought alloys for robust product design and durability assurance, a finite element based approach was developed by coupling a nodal-based transient heat transfer algorithm with material thermo-viscoplastic constitutive model. The integrated residual stress model has demonstrated its robustness in predicting residual stresses and optimizing heat treatment of aluminum wrought alloys.

**3:15 PM**
**Finite Element Study of the Aluminum AA6111T4 Blanking Process and Its Influence on Sheet Stretchability**: *Xiaohua Hu*[1]; Dong Mhung Suh[1]; Kyoo Sil Choi[1]; Xin Sun[1]; Sergey Golovaschenko[2]; [1]Pacific Northwest National Laboratory; [2]Ford Research and Advanced Engineering

Traditional and advanced blanking of AA6111T4 Al sheets were studied by plane strain FE models with damage parameters estimated from experimental fracture surface grain aspect ratio observations. Tension simulations were performed on 3D models with schematic or predicted cutting edge damages from blanking to investigate the effect of those damages on stretchability. The simulation for traditional blanking show that cracks initiate at the blank outside the fillet of the upper trimming tool corner which tends to loose contact with the tool. The crack opening necessitates the rollover of the tool over the fillet indent feature and leads to sliver formations. The burr size increases with blanking clearances. The simulations for advanced blanking with scrap support and dull upper trimming tool show that the crack initiation location has shifted to the sharp corner of the lower trimming tool, leading to the burr formation on the scrap side and much better quality on the part side which will be used in the following forming operations. The fracture surfaces become more tilted and the tilting angles increase with clearances up to 32% and decrease at 43%. The angles are similar for the clearances of 43% and 60% respectively. The conclusions observed in these simulations are all in line with experimental observations. The results of tensile stretchability results are similar to those of experiments in terms of influences of cutting clearances on both the failure modes and the elongations in the tensile strechability tests.

**3:35 PM**
**Effects of Pore Distribution Features on Ductility of Mg Castings**: *Kyoo Sil Choi*[1]; Xin Sun[1]; Dongsheng Li[1]; Mei Li[2]; John Allison[3]; [1]PNNL; [2]Ford Motor Company; [3]University of Michigan

Mg castings have found increasing applications in lightweight vehicles because magnesium and its alloys are the lightest metallic structure materials. However, a critical technical hurdle hindering the wider applications of Mg castings in vehicle applications is its limited ductility. Previous studies have demonstrated that, among various microstructural

features influencing the ductility of Mg castings, the extrinsic defects (i.e., porosity) are the dominant ductility limiting factor for the samples with porosity volume fraction exceeding a critical value. In this study, the effects of large-size pores and their locations on the ductility of Mg castings are evaluated based on two-dimensional microstructure-based finite element modeling methods. For this purpose, a series of synthetic microstructures are first generated such that they have different large-size pores and relative locations within the generated microstructures. Pores are explicitly represented in the synthetic microstructures and meshed out for the finite element based analysis. In the finite element-based ductility analysis, an intrinsic critical strain value of 14% is used for the Mg matrix, beyond which there is no work hardening. With no artificial failure criterion prescribed, different ductility levels are predicted for the various microstructures in the form of strain localization. The effects of microstructure size on the ductility are also evaluated by considering different-size microstructures. The predicted ductility is compared to each other based on the different microstructural features (i.e., pore size, location, RVE size and local pore volume fraction).

**3:55 PM**

**Phase-field Simulations of Grain Growth in a Thermal Gradient**: *Tao Jing*[1]; Qiwei Zheng[1]; [1]Tsinghua University

In this paper, the grain growth process in a thermal gradient is simulated with phase-field method in two dimensions. We get the relationship between tip velocity and undercooling first. Then the morphology of an equiaxed grain isolated in a thermal gradient is simulated. It's different from those in isothermal conditions, because the tip velocity varies with undercooling. We also investigate the competitive grain growth process in directional solidification with a great thermal gradient. The results present how the misaligned grain is eliminated in the competition with the well-aligned dendrites. An orientation variable is introduced into our phase-field model to distinguish different grains. It's more efficient than multi-phase-field models when the amount of grains is large, so this model is useful to simulate the grain selection process in single crystal turbine blade castings.

## ICME Applications: Ferrous

Monday PM Room: Ballroom E
July 8, 2013 Location: Salt Lake Marriott Downtown at City Creek

*Session Chairs:* Zi-Kui Liu, Pennsylvania State University; Warren Poole, University of British Columbia

**1:35 PM**

**An Integrated Computational Approach to Predicting the Transition from Internal to External Oxidation of Advanced Alloys in Extreme Environments**: *Zi-Kui Liu*[1]; Adri van Duin[1]; John Kitchin[2]; Andrew Gellman[2]; Brian Gleeson[3]; Guofeng Wang[3]; Michael Gao[4]; DeNyago Tafen[4]; Youhai Wen[5]; Dominic Alfonso[5]; Bryan Morreale[5]; David Alman[5]; [1]The Pennsylvania State University; [2]Carnegie Mellon University; [3]The University of Pittsburgh; [4]National Energy Technology Laboratory - URS Corporation; [5]National Energy Technology Laboratory

This effort describes a research consortium, composed of several nationally recognized academic institutions, an industry partner and a government laboratory, that is utilizing a multi-discipline team to accelerate the development of materials with tailored properties for the harsh environments consistent with future energy applications. Initially, the research is integrating computational and experimental approaches across various length and time scales to develop a predictive approach for describing the fundamental phenomenon dictating scale formation, as part of a long range goal of developing tool sets to predict materials performance and accelerate the design alloys for use in extreme environments. Advanced alloys for use in extreme environments rely on the formation of a passive oxide layer for environmental protection. A "minor" alloying constituent, such as Cr or Al provide environmental resistance to Fe-based stainless steel and Ni-base superalloys through the formation of protective $Cr_2O_3$ or $Al_2O_3$ scale and a critical amount is needed to promote external oxidation (continuous protective scale formation). Experimentally and in practice this critical amount is dependent on environment. In this presentation, Wagner's expression for this critical composition is examined through computational mean to determine underlining oxidation behavior of the Ni-Al-Fe system in the presence of various gases environments, including $O_2$, $H_2O$, and $CO_2$.

**1:55 PM**

**ICME Approach to Corrosion Pit Growth Prediction**: *Ken Smith*[1]; Lei Chen[1]; Rob Darling[1]; Mark Jaworowski[1]; Susanne Opalka[1]; George Zafiris[1]; Thomas Garosshen[1]; Sonia Tulyani[1]; [1]United Technologies Research Center

Corrosion is a significant problem in a large number of aerospace and commercial applications. Prediction of expected pit size and distribution due to localized corrosion processes is essential in understanding product life. Until now, the approach to predict pit size has been based on statistical analysis of pits in exposure tests. In this work, a combined experimental and multi-scale modeling method is used to develop a physics-based approach to understanding the factors that affect pit growth. The integrated approach uses thermodynamic modeling to understand the pit solution chemistry, atomistic modeling to study the kinetics, and experimental electro-kinetic measurements to validate the model predictions. Each of these pieces feed into an analytical model of pit growth to determine the maximum theoretical size. Model assumptions, results and pit size predictions for model aluminum systems will be presented.

**2:15 PM**

**Multiscale Model for Non-metallic Inclusions/Steel Composite System using Data Science Enabled Structure-Property Linkages**: *Akash Gupta*[1]; Ahmet Cecen[2]; Sharad Goyal[1]; Amarendra Singh[1]; Surya Kalidindi[3]; [1]TRDDC-TCS Innovation Labs, Tata Consultancy Services Ltd., [2]Department of Mechanical Engineering and Mechanics, Drexel University, [3]Woodruff School of Mechanical Engineering, Georgia Institute of Technology

Cleanliness is a major concern for steel manufacturers therefore, they constantly strive to modify and reduce non-metallic inclusions in the final product. Performance and quality of final steel sheet is strongly influenced by composition, morphology, type, size and distribution of inclusions in steel sheet. The aim of current work is to critically evaluate the versatility of a new data science enabled approach for establishing objective, high fidelity, structure-property correlations that are needed to facilitate optimal design of the processing path to realize enhanced performance of the final product. A 2-D finite element based micro-mechanical model was developed to simulate, the effect of various spatial configurations and geometries of hard and soft inclusions in a steel matrix system, on the final properties of processed sheet. From each microscale simulation five macroscale parameters - yield strength, effective hardening rate, localization propensity, average contact gap and plasticity index were extracted. A large number of microstructures were evaluated using micro-mechanical model, and for each microstructure a reduced-order representation was extracted using principal components of its 2-point statistics. These measures of the microstructure were then linked with the macroscale parameters listed above using regression methods. It is demonstrated that the data-driven, fully automated protocols developed in this study produce computationally efficient high fidelity linkages needed to facilitate process design. In particular, these linkages would prove valuable in designing hot and cold rolling operations through consideration of the acceptable level of inclusions that can be tolerated in the final product based on quality and processing requirements.

**2:35 PM Break**

**2:55 PM**

**Steel - Ab initio: Quantum Mechanics Guided Design of New Fe Based Materials**: *Ulrich Prahl*[1]; Wolfgang Bleck[1]; Alireza Saeed-Akbari[1]; [1]RWTH Aachen University

This contribution reports on the results of the SFB 571 "Steel - ab initio" that is a cooperation of the RWTH Aachen University and the Max-Planck- Institute of Iron Research in Duesseldorf (MPIE) financed by the Deutsche Forschungsgemeinschaft. For the first time it is exploited, how ab initio approaches may lead to a detailed understanding and thus to a specific improvement of material development. The challenge lies in the combination of abstract natural science theories with rather engineering like established concepts. Aiming at the technological target of the development of a new type of structural materials based on Fe-Mn-C alloys the combination of ab initio and engineering methods is new, but could be followed quite successfully. Three major topics are treated in this research unit: - Development of a new method for material- and process-development based on ab initio calculations. - Materialdesign of a new class of structural materials with extraordinary property combinations. - Acceleration of development time and reduction of experimental efforts and complexity for material- and process-development.In this presentation an overview of the first 5 years results will be given as well as an outlock for the upcoming 3 years periode.

**3:15 PM**

**An Integrated Model for Microstructure Development in the Heat Affected Zone of an X80 Linepipe Steel**: *Warren Poole*[1]; M. Militzer[1]; T. Garcin[1]; [1]The University of British Columbia

The integrity of pipeline welds is critical to the successful deployment of new capacity to transport natural gas and oil. This work is focused on a critical aspect of the pipeline, i.e. the heat affected zone (HAZ) of a multi-pass gas metal arc girth weld. The final mechanical properties of the HAZ are a complex function of the thermal history from welding. In particular, there is an intimate interplay between austenite grain growth, dissolution of Nb based precipitates and the subsequent decomposition of austenite. In this work, a phenomenological temperature model based on the Rosenthal equation has been integrated with microstructure sub-models for austenite grain growth, precipitate dissolution and austenite decomposition (including ferrite, bainite and martensite/retained austenite) for a selected X80 linepipe steel. The integrated model has been applied to a number of welding scenarios that have very different heat input conditions in order to predict the spatial variation of microstructure in the HAZ. In parallel, a preliminary model to link microstructure to mechanical properties has been developed. The overall model provides a tool to design optimized welding scenarios.

**3:35 PM**

**ICME Implementation for Steel Ingot Manufacturing & Conversion**: *Patrick Anderson*[1]; Stephanie Will[1]; E. Buddy Damm[1]; [1]The Timken Company

Virtual product engineering utilizing a chain of computational materials engineering software tools made critical contributions to the preparation, start-up and process optimization activities in support of Timken's new in-line forge press installation. These tools, taking advantage of the latest computationally efficient workstations, have been used to simulate processes previously too complex to model in an industrially relevant timeframe. Of primary interest is tracking key quality indicators throughout the entire ingot to bar manufacturing process path. Casting simulation software was used to simulate filling and solidification of bottom-poured steel ingots. Custom post-processing programs were written in order to collect the key outputs of interest and to create inputs for heat treat and deformation modeling. Deformation modeling, both open-die forging and rolling, was conducted in order to compare and contrast the varying process paths with respect to equivalent final product quality. Material model results were calibrated and validated using historic data and new in-plant measurements in order to serve as better predictive tools. Utilization of the virtual manufacturing chain allowed for increased efficiency in preliminary product trials, validation (or refuting) of process modification hypotheses and identification of subsequent process and product optimization opportunities.

**3:55 PM CANCELLED**

**Finite Element Modeling of Gear Hobbing and Milling**: *Troy Marusich*[1]; Deyao Ren[1]; Shuji Usui[1]; Jon Wadell[1]; Wenyang Liu[1]; [1]Third Wave Systems

Current processes for producing transmission gears involve hobbing, milling or shaping of a forged stock to obtain the gear shape. The amount of residual stresses, distortions, and excess material generated during hobbing and following heat treatment processes dictate overall cycle times and component performance. It is desirable for tooling designers and manufacturing engineers to have a physics-based modeling tool for gear cutting. In this paper, details are provided for a finite element-based model of gear hobbing and milling processes. The model explicitly meshes gear cutter geometries and simulates the complicated kinematic motion between tool and workpiece. In addition, the complex geometry of involute tooth profiles results in complicated contact scenarios on the evolving workpiece geometry during tooth profile generation. Furthermore, advanced adaptive meshing strategies are developed and employed to maintain the resolution of the tool-workpiece interaction while multiple teeth are in contact. Cutting forces, temperatures and stresses in the tool and workpiece are predicted for steel workpiece materials. Models are validated through a set of initially simplified experiments where incremental complexity is added, allowing for direct comparison between predicted and measured forces and chip shapes.

## Poster Session I: Modeling, Data and Infrastructure Tools

Monday PM Room: Ballroom AB&C
July 8, 2013 Location: Salt Lake Marriott Downtown at City Creek

**PI-1: 3D X-ray Diffraction Contrast Tomography Reconstruction of Polycrystalline Strontium Titanate during Sintering and EBSD Validation**: *Peter Gumbsch*[1]; B. Loedermann[2]; A. Graff[1]; A. Trenkle[2]; M. Syha[2]; D. Weygand[2]; W. Ludwig[3]; [1]Fraunhofer IWM; [2]Institute for Applied Materials IAM; [3]European Synchrotron Radiation Facility

A cylindric strontium titanate specimen that has been subjected to repetitive x-ray diffraction tomography (DCT) scans during sintering to follow the loss of porosity and grain growth. The specimen is also investigated by means of electron backscatter diffraction analysis (EBSD). Therefor, cross-sections of the sample have been prepared by mechanical polishing. Corresponding cross-sections of the reconstructed microstructure are identified and compared to EBSD characterization. Moreover, a 3D reconstruction of the destructive characterizations is presented and aligned to the structure as obtained by DCT alongside with a direct comparison of the crystallographic orientation obtained for the individual crystallites. Focussing on the position and curvature of the grain boundaries, the results are discussed in the context of spatial resolution and optimization potential for the reconstruction procedure of the diffraction data.

**PI-2: A Brief Review of Precipitation Hardening Models for Aluminum Alloys**: *Guannan Guo*[1]; Qigui Wang[2]; Gang Wang[3]; Yiming Rong[1]; [1]Worcester Polytechnic Institute; [2]GM-Global Powertrain Engineering; [3]Tsinghua University

Aluminum alloys are widely applied in structural applications for their lightweight, high strength and relatively low manufacturing cost. Most aluminum alloys used for critical structures are usually subjected to precipitation hardening. This paper briefly reviews the precipitation hardening simulations in aluminum alloys. Several well-accepted

hardening models are regenerated and discussed, comparing with experiment data of aluminum A356 alloy at various aging temperature. Based on the evaluation results of various models with the experiment data, further improvement of precipitation hardening models is considered. Key words: Precipitation hardening; Aluminum alloys; Heat treatment; Strengthening modeling

**PI-3: A Computational Method for Activation Energy Calculation using Non isothermal Conditions, Linear Heating Rate and Cubic Spline Interpolation Technique**: *Rabindranath Ray*[1]; [1]NIT DURGAPUR

The activation energy of $CaCO_3$ and $MgCO_3$ may undergo changes when subjected to different heating rates. Thermo-gravimetric measurements of mass loss for the sample is used under the assumption of a rate law for calculation of activation energy of these compounds. The fraction unreacted and temperature data is plotted by a cubic spline interpolation to generate a smooth curve. Activation energy of the compounds is then derived from this curve by regressional analysis. Prior to this, computational model is validated for correctness with data generated by a computer program for a reaction with known rate law and activation energy.

**PI-4: A Cross-slip Mechanism of Intermittent Plasticity in Nano- and Micro-pillars**: *Tamer Crosby*[1]; Nasr Ghoniem[1]; [1]UCLA

Currently, there is a great interest in the scientific community on the synergistic effects of the geometry and the initial microstructure on both the strength and the post-yielding behavior of FCC materials. For instance, it is well known from micro-tensile and nano-indentation experiments that the smaller the diameter of the pillar becomes, the higher its yield strength. This apparent size effect depend on both the evolution of the internal dislocation microstructure (intrinsic effect) and the finite dimensions of the sample which amplifies the importance of the interaction between dislocations and external surfaces (extrinsic effects). Although a vast literature exists on the role of different mechanisms on the strengthening of micro- and nano-pillars, few exist on the hardening/softening course that follows after the initial yield point. Here, we performed three-dimensional dislocation dynamics simulation, coupled to a boundary value problem through finite element analysis, on micro- and nano-pillar in order to investigate the relation between the microstructure and the post-yielding hardening. In this work we introduce a cross-slip mechanism for plasticity in pillars. It was observed that one of the main roles of cross-slip is the formation of dipolar-loops which affect the characteristics of the stress-strain relation of the material. The physics of this mechanism are similar to the idea of "stick-slip" behavior, where dipolar-loops shrink to a minimum size, before expanding again at a new critical stress.

**PI-5: A Machine Learning Framework for Efficient EBSD Microscopy Applied to AZ31**: *Travis Rampton*[1]; David Fullwood[1]; [1]Brigham Young University

While machine learning methods have been extensively applied in many areas of technology, they are still relatively under-utilized in the field of materials science. Such methods are particularly relevant to characterization methods, such as electron backscatter diffraction (EBSD) where large amounts of data are generated, and interpretation of underlying physics depends upon correct and efficient interpretation of the data. In this paper we apply machine learning approaches to both enhance the efficiency of EBSD characterization methods, and to extract physics from the subsequent data. The framework is demonstrated for a typical rare-event situation, in the form of twin nucleation in AZ31 magnesium. Not only does the researcher wish to find correlations between local structure and nucleation events, but this information should then ideally be used to guide the microscopy in the efficient search for future events. In this study, machine learning will be used to capture cause and effect of physical phenomena in the form of a decision tree at each relevant length-scale (grain, grain boundary (GB), and localized regions on GBs) via post-processing of high resolution EBSD data. The machine learning process will rank dominant structure and local field attributes at each level. The resulting knowledge will subsequently be used to identify zones of potential twin nucleation for efficient search of further events using the microscopy characterization tools. The positive feedback loop will lead to a combined computational-characterization framework for the study of critical events and multi-scale problems in material science

**PI-6: A Multi-scale Model to Simulate Forming Limit Diagram of Aluminum Sheets**: *Kaan Inal*[1]; Abhijit Brahme[1]; Raja Mishra[2]; [1]University of Waterloo; [2]General Motors Research and Development

This poster will highlight a multi-scale computational approach involving coupled micro-scale and macro-scale numerical models to simulate the forming limit diagram (FLD) of aluminum alloy sheets and facilitate faster their engineering application by bypassing costly experimental measurements. For the micro-scale computation, a new 3D finite element analyses based on rate-dependent crystal plasticity theory is developed that incorporates 3D microstructure constructed from 2D electron backscatter diffraction (EBSD) data into FE analyses. The numerical analysis accounts for the evolving crystallographic texture as well as 3D grain morphologies. A unit cube approach is adopted where an element or number of elements of the finite element mesh are considered to represent a single crystal within the polycrystal aggregate. Furthermore, a new hardening model is employed in the constitutive law to accurately account for changes in material at the microscale during forming under complex strain paths. Dislocation creation/annihilation, mean slip distance and deformation cell formation are accounted for in this formulation, permitting strain hardening and saturation not to be adjusted externally. This approach also eliminates the use of an artificial imperfection as used in the M-K based models to predict FLDs since localized deformation occurs as a natural outcome in this approach. Simulations of FLDs are performed with the numerical model and the effects of various macroscopic (strain paths, etc.) and microscopic (dislocations cell structure, etc.) phenomena on the limit strains are investigated. The predictions are compared to experimental FLDs when available to validate the approach and build the model as a robust engineering tool.

**PI-7: A Three-dimensional Lattice Boltzmann Model for Columnar Dendrite Growth**: *Mohsen Eshraghi*[1]; Bohumir Jelinek[1]; Sergio Felicelli[1]; [1]Mississippi State University

A three-dimensional (3D) lattice Boltzmann (LB) model is developed for simulating columnar dendritic growth in a binary alloy. The growth kinetics is controlled by solute and temperature distributions around the dendrite. Melt convection can also alter the kinetics of solidification by washing the solute away from the solid/liquid interface. LB is used to solve for fluid flow, mass, and heat transport, whereas cellular automaton (CA) is employed to capture the interface. The evolution of multiple 3D columnar dendrites under the effect of melt convection is investigated. It is shown that convection can change the kinetics of growth by affecting the solute distribution around the dendrites. Considering the local characteristics and parallel scalablility of the LB and CA methods, the present model can be used as a new tool for 3D simulation of columnar dendritic solidification under melt convection.

**PI-8: Building 3D Microstructure Database using an Advanced Metallographic Serial Sectioning Technique and Robust 3D Segmentation Tools**: *Umesh Adiga*[1]; Murali Gorantla[1]; James Scott[1]; Daniel Banks[1]; Yoon-Suk Choi[1]; [1]UES, Inc

Building a 3D microstructure database is gaining rapid attention as it provides a materials key knowledgebase toward ICME approaches. Recent advances in automated metallographic serial sectioning technique such as RoboMet.3D, has significantly improved metallographic procedures and control systems for the acquisition of quality metallographs from serial sections. However, the image registration for 3D reconstruction and the segmentation of actual microstructural attributes from the raw data still remain as challenging issues, particularly for polycrystalline materials. The present study demonstrates systematic efforts to improve the automated metallographic serial sectioning technique for the controlled 3D microstructure data. In particular, comprehensive post-processing tools were developed for the segmentation of complex 3D raw microstructures. These tools were based upon advanced image processing algorithms targeting different types of microstructures. Its capability of handling various complex 3D microstructure data (from polycrystals to composites) is also demonstrated. Geometric and gray-scale features are calculated using voxel values and their scale-space relational analysis. We propose to build a volumetric image database that allows qualitative and quantitative comparison of different materials and their structural properties as measured by image processing algorithms.

**PI-9: CALPHAD File Repositories: Increasing Efficiency and Reproducibility**: *Carelyn Campbell*[1]; Ursula Kattner[1]; Laura Bartolo[2]; [1]National Institute of Standards and Technology; [2]Kent State University

The CALPHAD method, which develops multicomponent composition, temperature, and pressure dependent functions based on unary, binary, and ternary descriptions, is a critical tool in integrating processing-structure and structure-property relationships. The development of a CALPHAD-based file repository is essential for increasing the efficiency and reproducibility of CALPHAD assessments for multicomponent thermodynamics, diffusion mobility, molar volume, and elastic properties. The file repository links functional descriptions (e.g. TDB files) and evaluated data files (e.g. POP files) and allows the files to be described using tags defining the file authors, the system constituents, the phase-based property of interest, the phases and other properties of interest. The platform for the file repository is scalable and extensible and enables users to enter data and associated metadata, to define a data citation for the upload data, to manage data permissions and to search for desired data.

**PI-10: Coupled Composition-Microstructure Modeling of a U-Pu-Zr Fuel**: *Jordan Cox*[1]; Eric Homer[1]; Veena Tikare[2]; [1]Brigham Young University; [2]Sandia National Laboratories

Solid state diffusion, irradiation and phase transformation drive the redistribution of constituents and microstructural coarsening in metallic alloys. Constituent redistribution can cause a previously homogenous alloy to become inhomogeneous, thus altering the physical and mechanical properties of the alloy. U-Pu-Zr is an alloy used in breeder reactors and experiences a redistribution of constituents in the presence of a thermal gradient. Irradiated fuel rods show three concentric zones with varying concentrations of constituents in each zone. The application of the Potts-phase field method, a coupling of the Potts Monte Carlo and phase field methods, to model the redistribution of constituents in the ternary alloy U-Pu-Zr is presented. The method focuses on diffusional fluxes of the different constituents as determined from gradients of the chemical potentials. The chemical potentials are in turn obtained from a thermodynamic database of the alloy. Details of the model application to the U-Pu-Zr system, as well as the physical parameters necessary to accurately model the system, are detailed. Finally, the entire process is discussed in the larger framework of Integrated Computational Materials Engineering.

**PI-11: Creating an Integrated, Community-Sourced, First-Principles Data Repository**: *Richard Taylor*[1]; Benjamin Burton[1]; Laura Bartolo[2]; [1]NIST; [2]Kent State University

As the quantity of materials computation surges, there is a pressing need for a reliable and standard framework for community-sourced data storage and indexing. Metadata standards and protocols are needed to index and make searchable pre-existing data repositories alongside such data. While paper and ink publication is, in many cases, not a suitable format for presenting or accessing data input and output, a properly designed repository functions as a tool to i) facilitate reproducibility of calculations, ii) provide access to computed results for reuse, extension and peer-review, and iii) significantly reduce the need to perform redundant computations. The First-Principles Phase Stability Repository is part of a concerted effort to develop such a framework. The repository itself comprises images, input and output source files, and reference data. It is flexible enough to accommodate virtually any file format. Efforts toward establishing communication and links between existing (and in many cases distinct) repositories are ongoing.

**PI-12: Crystal Plasticity Finite Element Modeling of Single Crystal Niobium Tensile Tests with Weighted Dynamic Hardening Rule**: *Aboozar Mapar*[1]; Thomas Bieler[1]; Farhang Pourboghrat[1]; Christopher Compton[1]; [1]Michigan State University

Fine grain Niobium (Nb) sheets are used to make superconductive cavities, which are the fundamental building blocks of particle accelerators. Slices of large grain Nb cut from ingots are cheaper to produce than fine grain sheets; however they are more prone to anisotropy. Reproducible manufacturing of a cavity with large grain (anisotropic) Nb sheets may be less expensive but it needs greater care in designing the complex strain paths required to plastically transform the Nb sheet into an accelerator cavity. An alternative to the trial-and-error method of manufacturing, that also reduces cost, is to use Integrated Computational Materials Engineering (ICME) techniques. ICME requires using a constitutive material model to predict the behavior of Nb sheet during the manufacturing operation. This constitutive model can then be implemented into a finite element code and used to design and optimize the manufacturing process. The premise of ICME for Nb sheet is to successfully model the behavior of a single crystal of Nb. If successful, the single crystal theory can be extended to model the behavior of polycrystals. In this research, we have developed a crystal plasticity code for a single crystal and implemented it into ABAQUS commercial FEM software. This code is able to accurately predict the shape change of an Nb single crystal, although is not as successful in predicting the stress history. To remedy this problem, we have modified the classical definition of the hardening rule for a single crystal. This modification helped the model to give better stress predictions.

**PI-13: Data Science Enabled Structure Property Correlation for Dual Phase Steel**: *Prabhash Kumar*[1]; Akash Gupta[1]; Sharad Goyal[1]; Amarendra Singh[1]; Surya Kalidindi[2]; [1]TRDDC, Tata Consultancy Services; [2]Georgia Institute of Technology

Robust structure-property correlations are critical for successful design and use of materials. Conventionally, the microstructure has been depicted by average grain size, phase fractions, pearlite spacing, etc. in these correlations. This depiction of microstructure is grossly inadequate for new materials with complex microstructure such as advanced high strength steel (AHSS). In this work our focus is to deploy statistical methods to analyse published microstructure and their corresponding properties for dual phase (DP) steel, one of the advanced high strength steel, and establish robust structure-property correlations. A large number of microstructures and their corresponding properties (YS, UTS, %Elongation etc.) for dual phase steel have been collected from published literature. Through image processing techniques different phases in microstructure are identified. These segmented microstructures are represented using principal components of their 2-point statistics. Further, regression method has been deployed to correlate these principal components with the above mentioned properties. It has been observed that microstructures belonging to different group of dual phase (DP) steel like DP 450, DP 600, DP 780 etc. can be segregated in the principal component space. Moreover, it is demonstrated that the

statistical approach developed in this work establishes robust correlations to link structure and properties. The proposed approach can help reduce the experimental requirements of material characterization, and the developed models linking structure with properties can be used in ICME framework for accelerated development of material.

**PI-14: Determination of the Characteristic Sizes of Complex Microstructures and Its Application to the Design of Composite Materials**: *Victor Chan*[1]; James Dempsey[1]; Katsuyo Thornton[1]; [1]University of Michigan, Ann Arbor

Intricate three-dimensional (3D) bicontinuous microstructures are well suited for multifunctional composites because they can accommodate different materials with complimentary properties. Triply-periodic minimal surfaces (TPMS), one class of 3D bicontinuous structures, has been theoretically shown to optimize transport and mechanical properties when the materials of the two phases exhibit competing properties. Using recently developed topological characterization methods that determine the size distributions of structural features in complex microstructures, we find that transport in TPMS is correlated with the ratio of the characteristic sizes of the channels and the nodes of their underlying structure; more specifically, we find that a characteristic channel to node size ratio of near unity is optimal. We also study mechanical properties of TPMS and use the relationships developed between the material properties and size of structural features to evaluate a self-assembled bicontinuous structure that results from spinodal decomposition, as well as experimentally obtained microstructures of a Lithium-ion battery cathode and a solid oxide fuel cell electrodes.

**PI-15: Dislocation Density Based Crystal Plasticity Finite Element Model of Polycrystals with Grain Boundary Effect**: *Zhe Leng*[1]; Alankar Alankar[2]; David Field[1]; Nathalie Allain-Bonasso[3]; Francis Wagner[3]; [1]Washington State University; [2]Los Alamos National Laboratory; [3]University of Metz

Grain boundaries play a important role in determining the mechanical properties of metallic materials, they provide a strengthening mechanism by impeding the dislocation motion. However, modeling the interaction between the dislocation and the grain boundaries in polycrystalline materials in a physically consistent way is still a long-standing, unsolved problem. In this study a dislocation density based crystal plasticity finite element model is applied to incorporate the interaction between the dislocations and the grain boundaries. The dislocations are in the form of closed loops and are tracked as an internal state variable. The evolution of geometrically necessary dislocations includes the non-zero flux divergence, and geometric reactions, while the evolution of statistically stored dislocations includes annihilation and generation. The grain boundaries in the model are represented by the bi-crystal volume elements, each having the crystallographic lattice orientations of its adjacent crystals. The grain boundary effects are considered on those near boundary bi-crystal volume elements by introducing an additional energy barrier for the dislocation motion. The simulation is conducted on a polycrystalline ferrite specimen under uniaxial tension, with 12% strain to check the GNDs distribution. The results indicate that the grain boundaries are favored by the GNDs, and the dislocation concentration at certain grain boundaries are alleviated by the slip transmission process.

**PI-16: Effect of Primary $Al_3Sc$ Particles on Fatigue Behavior Studied through Experimentation and Simulation**: *Nilesh Kumar*[1]; Mageshwari Komarasamy[1]; Rajiv Mishra[1]; [1]University of North Texas

The presence of primary $Al_3Sc$ particles enhances both the crack initiation and propagation tendencies and hence affects the fatigue life on both the regimes. The effect of coarser $Al_3Sc$ particles and clusters on fatigue behavior of an Al-Mg-Sc alloy was studied through experiments and finite element (FE) simulations. The accumulation of strain around the particles was studied as a function of particle and cluster size, and the mean distance between the particles and/or clusters. The possible and favorable crack initiation sites around the particles were identified based on accumulated plastic strain using FE analysis. The crack propagation characteristics in the matrix containing elastically stiff ($Al_3Sc$) particles were also studied. Fractured surfaces were characterized using scanning electron microscopy to further understand the crack initiation, propagation and their correlation with the primary particles.

**PI-17: Establishing the Ni-Fe-Cr-Al-O Thermodynamic Database: DFT Calculations, CALPHAD Modeling and Experiments**: *Bi-Cheng Zhou*[1]; Michael Gao[2]; ShunLi Shang[1]; Cuiping Guo[1]; Ömer Dogan[3]; Zi-Kui Liu[1]; [1]The Pennsylvania State University; [2]National Energy Technology Laboratory; [3]URS Corporation

In order to gain fundamental understanding of the degradation mechanisms of Ni- and Fe-based engineering alloys in coal-derived environment at high temperatures, a model quaternary Ni-Fe-Cr-Al system in environments of oxygen, hydrogen, water vapor, and carbon dioxide is chosen for multiscale computer modeling supported by experimental investigation at the National Energy Technology Lab-Regional University Alliance. Formation of continuous coherent Al2O3 scale on the alloy surface is the key to oxidation resistance of the alloys, which depends on the oxygen solubility and oxygen diffusion in the bulk alloys. Due to the lack of sufficient phase diagram information in the literature on the Ni-Fe-Al-Cr-O systems, an integrated approach that combines first-principles calculations based on the density functional theory (DFT), CALPHAD modeling, and experiments is adopted to accelerate the investigation of the phase equilibria and the development of a self-consistent thermodynamic database for the systems. Specifically, enthalpy of formation of oxides and their end-members and oxygen solubility in Ni are calculated using DFT methods. Phonon calculations are carried out to predict the free energies at finite temperatures of selected oxides. Experimental investigations of phase equilibria in oxygen are carried out at controlled temperature and pressure followed by phase identification using advanced electron microscopy and x-ray diffraction. Phase transition temperatures are measured using differential thermal analysis. DFT calculations and experiments provide reliable thermochemistry and phase equilibrium data as input to and thus expedite the optimization scheme of CALPHAD modeling. The initial focus is put on Ni-Fe-Al-O, and then effort is extended to Ni-Fe-Cr-Al-O system.

**PI-18: Fracture Mode of a Ni-based Single Crystal Superalloy Containing Topologically-Close-Packed Phases at Ambient Temperature**: Qianying Shi[1]; Xianfei Ding[1]; Yunrong Zheng[1]; Jingyang Chen[1]; *Qiang Feng*[1]; [1]University of Science and Technology Beijing

High levels of refractory alloying elements (such as Mo, Re and W) in modern Ni-based single crystal superalloys increase the tendency of microstructural instability, especially the precipitation of topologically close packed (TCP) phase. Most of previous research mainly focused on the composition, morphology, precipitation and growth behavior of TCP phases in Ni-based single crystal superalloys, whereas there were limited reports about their role on fracture features. In this study, a simple and practical method at ambient temperature was developed to understand the specific effect of TCP phases on the fracture mode. Small scale specimens of a single crystal superalloy containing different amount of TCP phases were investigated. Microstructural investigation and compositional analyses by Auger electron spectroscopy were performed on the matching fracture surface after impact tests. It is suggested the fracture mode related to TCP phases occurred in two ways: 1) the interfacial decohesion between TCP and enveloped γ' phase due to the weak TCP/γ' interface coherency and 2) the spallation of TCP phase itself. Fracture modes of investigated specimens were associated with the number of TCP phases. Moreover, different fracture microstructures were observed in specimens with and without TCP phase, respectively, and their fracture modes were discussed. This work is supportive for the relevant investigation at high temperature, although the impact test was carried out at room temperature. Understanding the role of TCP phases playing in the fracture process is also significant to clarify the creep and fatigue mechanism at high temperature in superalloys containing TCP phases.

**PI-19: Interaction of Point Defects with Twin Boundaries in Au: A Molecular Dynamics Approach**: *Babar Khan*[1]; [1]Central China Normal University

Some low index (111), (113), and (120) twin-boundaries in Au at various temperatures are calculated using molecular dynamics simulation technique with many-body and semi-empirical potentials, based on the embedded atom method developed by Daw and Baskes. The considerable relaxations are found on both sides of (113), and (120) interfaces with same magnitude, except around (111) interface due to high atomic density of (111) plane. Interactions of single-, di- and tri-vacancy with twin interfaces at 300 K are calculated. Vacancy clusters are also checked on mirror and off-mirror sites. All vacancy clusters are favorable on mirror arrangement near (113) twin-boundary. Single- and di-vacancy are more favorable on mirror site near (111) twin-boundary, while these are attractive on off-mirror sites near (120) twin-boundary. All vacancy clusters (averagely) are more favorable at closest planes as compared to away from the interface, except tri-vacancies near (120) interface on off-mirror site and cluster 3.3 and 3.4 on both sites near (111) interface which are favorable away from the interface. The effect of temperature on interaction behavior shows that interaction energy is increased with the increase of temperature, except for single-vacancy near (111) interface.

**PI-20: Investigation of γ' Precipitation in Ni-base Superalloy PWA1480 by Interrupted Cooling Coupled with Thermo-kinetic Simulation**: *Erwin Povoden-Karadeniz*[1]; Markus Kozeschnik[2]; Ernst Kozeschnik[3]; [1]Vienna University of Technology; [2]Graz University of Technology; [3]Vienna University of Technology, Institute of Materials Science and Technology

Interrupted cooling experiments are capable of discovering the start temperature, Tstart, of the earliest stages of precipitation. With this method, the start of $Ni_3Al$-type γ' precipitation in single-crystal Ni-base superalloy PWA1480 was determined inside 5 K. Solution-treated specimens were stepwise cooled to different temperatures above and below the estimated temperature, where nucleation of γ' occurred first. The microstructures resulting from these cooling experiments were explored by transmission electron microscopy. Development from initially cuboid, diffuse particles via octo-cubes towards octo-dendrites was shown as a function of interrupting temperature. Differential scanning calorimetry prior to the interrupted cooling experiments was used to identify the temperature range of the main event of γ' formation. The experimental heat flow, as well as particle size and distribution was reproduced in a thermo-kinetic precipitation simulation, when a diffuse interface between Ni-matrix and γ' precipitates was stated for the precipitates, which formed close to their solvus temperature. Best agreement of the simulation results with the experiments was obtained, when the interfacial energy was continuously approximated to the energy of a sharp interface with decreasing interrupting temperature.

**PI-21: CANCELLED: Micromechanical Stereoinference**: *Thomas Hardin*[1]; Brent Adams[1]; Eric Homer[1]; David Fullwood[1]; [1]Brigham Young University

Some crystal plasticity models make use of dislocation density knowledge accessible by Electron Backscatter Microscopy. However, current two-dimensional EBSD accesses only a 2-dimensional, incomplete distribution of dislocations. A novel computational method of micromechanical stereoinference is reported which yields components and gradients of Nye's GND tensor. The method overcomes limitations imposed by metal's electron opacity by combining experimentally-accessible Nye's tensor components and measured infinitesimal elastic distortion tensors with a solution to the underlying stress equilibrium equations. A computational validation scheme for that method is presented and is shown to be largely robust to random experimental error. It is expected that the added knowledge of the full Nye's tensor will improve strain-gradient plasticity models, and thereby improve the necessary tools for Integrated Computational Materials Engineering.

**PI-22: Multi-physics, Multi-scale Simulations of MEMS with Quantified Uncertainties**: *Alejandro Strachan*[1]; [1]Purdue University

I will present a multi-physics, multi-scale model to predict, with quantified uncertainties, the performance of a radio frequency capacitive MEMS switch developed by the PSAAP Center for the Prediction of Reliability, Integrity and Survivability of Microsystems. The device of interest is as electrostatically actuated contacting switch and its performance is governs by a complex coupled physics involving solid mechanics, dielectric charging, fluid damping and contacts between solid surfaces with nanoscale asperities. We describe the switch in terms of its chemistry, nanostructure, and geometry within a Bayesian framework that appropriately accounts for uncertainties of disparate origin, from the intrinsic device- and atomic-level variability to model-form and numerical errors. The full-physics device-level simulations are informed by a combination of: i) first-principles multiscale models; ii) direct experimental measurements; and iii) calibration experiments on a variety of devices; and is used to predict operating parameters of the device of interest and their degradation. Our models quantify how geometrical, nanostructural and atomic level variability affect device performance highlighting the complex coupling of scales and physics in microdevices. A Bayesian validation approach is used to quantify the confidence in the model based on experimental data. Such analysis is critical for modeling-based decision-making in materials and device design.

**PI-23: Multiscale Computational Modeling of Adsorption**: *Adam Donato*[1]; Ranga Pitchumani[1]; [1]Virginia Tech

Computational modeling of materials and associated phenomena typically relies on empirical data for various properties, ranging from macroscale properties (e.g. thermal conductivity) to nano-scale properties (e.g. bond lengths). In particular, a comprehensive materials modeling effort involves describing multiscale phenomena at a cascade of length and temporal scales, which presents a bewildering computational challenge. In an effort to effectively bridge the modeling across the various length scales from the atomistic to the macroscale, this paper presents a computationally efficient method of predicting materials properties by starting from *ab initio* quantum chemistry techniques alongside molecular modeling. The method is demonstrated on the analysis of alkanes adsorbing in the crystal structure of zeolites. The multiscale methodology requires only the chemical composition of the alkanes and zeolites (e.g. the number of each element involved) from which we were able to determine the chemical structure of the alkanes and zeolites, as well as macro-scale properties including the heat of adsorption, adsorption equilibrium isotherms, and alkane diffusivities. The results are quantitatively validated against empirical data. The work done with adsorption has immediate applications for chemical separations, such as carbon capture and catalytic cracking, as well as the low pressure storage of natural gas or hydrogen. This multiscale analysis can also be used in the development and analysis of new metal-organic framework adsorbents, or other novel adsorbent materials. And this technique can also be extended beyond adsorption to be used in the analysis of structural properties, temperature effects, biological interactions, or other systems involving multiscale behavior.

**PI-24: CANCELLED: Numerical Simulation of Sintering in the Ceramic Oxide**: *Mohammed Kadhim*[1]; Adill Alwan[2]; Elham Ibraheem[2]; [1]University of Technology; [2]University of Babylon, Babylon, Iraq

Sintering process has been analyzed mathematically by prediction unsteady-state mathematical model in order to give more description and understanding for the mechanism of this process. This includes mass transport phenomena occur via diffusion. The spatial and temporal temperature profiles with the solid medium has been determined by solving the unsteady state Fourier heat energy transport equation using the explicit finite difference numerical method which would minimize the solution errors. This has been more realistic determination of temperature distribution within the work-piece. Alumina has been selected as a target to represent nonmetallic material of diverse physical and thermal properties. The average grain size for alumina powder is 0.5 μm with initial compact

density 2160 kg/m3. These values gave a reliable approach to calculate the porosity and relative strength.

**PI-25: Phase Field Modeling of Metal Oxidation Behavior**: Tianle Cheng[1]; *Youhai Wen*[2]; [1]ORISE; [2]National Energy Technology Laboratory

Accurate prediction of oxidation kinetics is essential to the life prediction of high temperature materials. Oxidation process involves mass diffusion and chemical reaction with the diffusing species usually charge carriers. Existing theoretical models are not applicable when the space charge effect becomes significant, which usually occurs when the oxide scale thickness falls in the range from nanometers to micrometers. To bridge this gap, a phase-field model is developed that takes into account the chemical reaction and charge-carrier diffusion in complex media with inhomogeneous dielectric constant, a very important feature as heterogeneity is common in oxide films with voids, micropores and cracks. Application of this model has captured the transition of rate-limiting process in oxide growth kinetics without any a prior assumption. The simulation also clearly reveals the roles of charge interaction and interplay between Debye length, film thickness and the resultant effective diffusivity.

**PI-26: Phase Formation and Kinetics during Aluminization of Nickel and Nickel-Chromium Wires**: *Thomas Philippe*[1]; Peter Voorhees[1]; Dinc Erdeniz[1]; David Dunand[1]; [1]Northwestern University

Aluminizing of Ni or Ni-Cr is mainly used to create thick coatings of intermetallic compounds. The goal of the process is to achieve a target Al composition in the wire in order to reach a particular equilibrium state after annealing. During pack aluminization process, Al is supplied to the wire surface through the vapor phase and diffuses in the sample involving the formation of three or four intermetallic compounds that leads to a complex multiphase inter-diffusion problem. We have used a phase field approach developed by N. Moelans to model both processes. The phase field approach allows for both bulk-diffusion controlled and interface-limited kinetics, as well as non-axisymmetric diffusion processes. The model employs composition-dependent Gibbs energies and mobilities optimized according to the CALPHAD method. The code is verified by comparing aluminization kinetics in Ni-Al and the unusual phase formation and dissolution process that occurs during homogenization of a multiphase wire. We then examine phase formation in the ternary Ni-Cr-Al system. We also find interfacial instabilities during inter-diffusion in simulations in Ni-Cr-Al that lead to an unexpected microstructure. More generally, this work demonstrates that this phase field formulation is a powerful tool for mesoscale computations of multiphase inter-diffusion problems in multicomponent systems.

**PI-27: Precipitation Simulation of AZ91 Magnesium Alloys**: *Chuan Zhang*[1]; Weisheng Cao[1]; Shuanglin Chen[1]; Jun Zhu[1]; Fan Zhang[1]; [1]CompuTherm LLC

Precipitation-hardening magnesium alloys have recently received an increasing interest for potential high-strength applications in the automotive, aircraft, aerospace, and electronic industries. The strength of magnesium alloys are mainly due to the solid-state precipitates that are produced by an age-hardening process. However, the precipitation phenomena in these alloys, especially in the very early stage of the precipitation process, are still far from being well understood, and many fundamental issues remain unsolved. Pure experimental investigation on the precipitation-hardening process requires tremendous amount of work. Associated with the precipitation simulation, guidelines can be outlined for the rational design and development of higher strength magnesium alloys via precipitation hardening with much less experimental work. In this work, the precipitation simulation of AZ91 magnesium alloy is carried out by the PandatTM software module: PanPrecipitation. Combining the thermodynamic/mobility and precipitation databases, one can simulate the evolution of the continuous precipitation of γ-Mg17Al12 precipitate (such as volume fraction, average particle size and particle size distribution) using the built-in precipitation models, and predict the mechanical properties (micro-hardness, yield strength etc.) according to the developed age-hardening models. The simulated results of the AZ91 magnesium alloy show good agreement with the experimental data in the literature. The currently obtained kinetic parameters show rather good predictive capability within the assessed composition ranges.

**PI-28: Reducing the Microstructure Design Space of 2nd Order Homogenization Techniques Using Discrete Fourier Transform**: *Tim Ruggles*[1]; Travis Rampton[1]; Scott Rose[1]; David Fullwood[1]; [1]Brigham Young University

Volume fraction (1-point statistics) microstructure design techniques have been developed to the point where they may be used for optimization of material design in many practical situations. However, the resultant designs contain no geometrical information relating to the structure of the optimal material. More complicated 2-point statistics (which include first order geometrical information) have only been applied to a handful of simplified design situations due to the computational effort to search the many-dimensional design space. This study applies spectral techniques via discrete Fourier transforms to decompose the 2-point homogenization relations in order to 1) deconvolve the influences of material properties and structure on the calculated performance, 2) enable efficient calculation of convolution integrals, and 3) facilitate the reduction of the structure design space through the inclusion of only dominant terms in the Fourier expansion. This 2nd order homogenization method is compared with 1st order methods, and validated using finite element analysis. The new framework is then used to design an optimized two-phase composite microstructure for a selected set of elastic material properties near the theoretical bounds for the material, resulting in only 0.1-5.8% deviation from the desired properties. The reduced space included only 6 Fourier terms, with the search for optimal designs being undertaken via simulated annealing.

**PI-29: Research on Numerical Simulation of the Temperature Field of the Innovation Cathode Cells**: *Jiang YanLi*[1]; Yu Liang[1]; Feng Naixiang[2]; [1]College of Materials Science and Engineering, Guilin University of Technology; [2]School of Materials & Metallurgy, Northeastern University

The mathematical model of temperature field of the aluminum reduction cell was established in the paper. The temperature field of the 160kA conventional and innovation cathode cells (with lower the anode-cathode distance) was numerically calculated with commercial software ANSYS. The calculated results of the 3D temperature field showed that: the simulated data was consistent with the measured results, the innovation cathode cells was cooler because of the bad insulation work of the bottom carbon block, and after redesigned, the bottom temperature of the innovation cathode cells was hearth.

**PI-30: Screw Dislocations Cores in Bcc Transition Metals: The Influence of Alloying and Temperature**: *Lorenz Romaner*[1]; Hong Li[2]; Claudia Ambrosch-Draxl[2]; Reinhard Pippan[3]; [1]Materials Center Leoben; [2]Humboldt-Universität zu Berlin; [3]Erich Schmid Institute

Dislocations are the carriers of plastic deformations and are, as such, key factors for the mechanical properties of materials. A dominant role for plastic deformation in bcc metals is assigned to ½<111> screw dislocations. Due to their non-planar core, these dislocations have low mobility and, therefore, limit plastic deformation in bcc metals. The properties of the core can be influenced via alloying [L. Romaner et al. Phys. Rev. Lett. 104, 195503 (2010), H. Li et al. Acta Mater. 60, 748 (2012)] and are of critical importance for the design of mechanical properties of bcc metals. We present calculations on ½ <111> screw dislocation cores in bcc transition metals based on density functional theory. Emphasis is given to the effects of alloying elements and effects of temperature. Alloying elements in random solution modify d-band occupancy and introduce local distortions. By means of supercell calculations containing up to 1000 atoms we show how these factors affect core structure and the topology of the dislocation line. Furthermore, the effects of temperature on the dislocation core are investigated on the basis of inter-string potentials and a thermodynamical approach involving evaluation of vibrational entropy. The bcc metals under investigation are W, V and Fe.

**PI-31: The Simulation as Prediction Tool to Determine the Method of Riser Calculation More Efficient**: *Lazaro Suarez*[1]; Norge Coello[1]; Alexis Alonso[1]; [1]UCLV

The riser must be adequate to satisfy the liquid and solidification shrinkage requirements of the casting. In addition, the riser itself will be solidifying, so the total shrinkage requirement to be met will be for the riser/casting combination. The total feeding requirement will depend on the specific alloy, the amount of superheat, the casting geometry, and the molding medium. The shape of a casting will affect the size of the riser needed to meet its feed requirements for the obvious reason that the longer the casting takes to solidify, the longer the riser must maintain a reservoir of liquid metal. A variety of methods have been devised to calculate the riser size (shape factor method, geometric method, the modulus method) needed to ensure that liquid feed metal will be available for as long as the solidifying casting requires. In this research has been calculated the riser geometry by different methods for a piece type wheel and the simulation has been used to determine which of the methods it is more efficient.

**PI-32: Towards the Interface Level Understanding of Internally Oxidized Metal-oxide Composite Cu-$Al_2O_3$**: *Yong Jiang*[1]; Guoqiang Lan[1]; Canhui Xu[1]; [1]Central South University

We report a systematic strategy for characterizing the interface-level microstructure evolution in metal-oxide composites during fabrication from first principles interfacial thermodynamics and classic kinetics analyses. This is demonstrated for the technologically important Cu-$Al_2O_3$ composite fabricated by in-situ internal oxidation. First, equilibrium atomic structures and corresponding energetics and properties of Cu-$Al_2O_3$ interfaces were determined from the first principles, as a function of temperature and the ambient oxygen partial pressure. The results were then used to construct the interface phase stability diagrams. Thermodynamic equilibrium solubilities and diffusion kinetics of oxygen in Cu matrix were further analyzed, to establish the connection between the ambient oxygen partial pressure and the local oxygen activity inside the composite. Finally we correlated the interface microstructures and adhesion properties of the internally oxidized composite with processing parameters during its fabrication.

**PI-33: Understanding and Predicting Fatigue Crack Growth from Physical Principles**: *Peter Huffman*[1]; Scott Beckman[1]; [1]Iowa State University

Metal fatigue remains one of the top causes of failure of structural components. The presented work will demonstrate a method to predict the fatigue behavior of ductile metals. The method combines fracture mechanics and atomic scale physics to predict quantitative fatigue crack growth rates. The strain distribution near a crack tip is approximated using a solution from linear elastic fracture mechanics. The theoretical strength of the crystal can be determined using density functional theory methods, by straining bonds until failure. The strain distribution is combined with the predicted theoretical strength to predict crack growth rate curves. To validate this approach the predictions generated for a variety of simple metals are compared to experimental data from literature. A demonstration of the use of the methodology going from the atomistic calculation to predict the fatigue life a component is presented.

**PI-34: Using of Automation in Generation of Engineering and Shop Drawings, and 3D Modeling in EPC Projects**: *Ali Soheilifar*[1]; Erfan Alavi[1]; [1]Sazeh Consultants

There are various methods in engineering, procurement, and construction regarding value engineering (VE) in a project, especially an EPC project, which are used by consulting and contracting companies. These methods are optimized and expanded frequently according to technology improvements and knowledge advancements. On the other side, the economical point of view has urged most of the companies to focus more on reducing the existing errors and an increase on productivity during a project. Therefore, the connection between the common design software's such as SACS and STAAD PRO, as well as obtaining three dimensional models, using PDMS with the assist of additional software's, has been investigated here. This has been done in order to make creating engineering drawings, construction, and producing the three dimensional model at the same time and in accordance with each other possible. This method has been practiced in petroleum, oil, and gas projects and an example is included in this paper. The results have shown that automation has reduced the time and cost, as well as an increase in accuracy and quality of the issued documents. In addition, automation has made implementing the changes made from reviews possible at all stages and in accordance with each other.

## Materials Data for ICME

Tuesday AM Room: Ballroom E
July 9, 2013 Location: Salt Lake Marriott Downtown at City Creek

*Session Chairs:* Carelyn Campbell, National Institute of Standards and Technology; Peter Collins, University of North Texas

**8:00 AM**
**Challenges and Approaches in Materials Data Management for ICME**: *Warren Hunt*[1]; Ross Brindle[1]; Scott Henry[2]; [1]Nexight Group LLC; [2]ASM International

Integral to the successful implementation of Integrated Computational Materials Engineering and realization of the goals of the Materials Genome Initiative is the availability of pedigreed, comprehensive data. A number of data–related issues are active topics of discussion in the materials community, with a variety of potential pathways to solution being proposed. One of those pathways is the establishment of the Computational Materials Data Network. This approach recognizes the unique needs of specific subgroups of data users in the community, and is developing separate "ecosystems" to address these different needs. This presentation will highlight the approaches used in the ecosystems that have been selected for initial development. In particular, it will focus on the aerospace materials ecosystem, which builds on the successful Materials Data Management Consortium, as well as an in-process materials processing and manufacturing ecosystem. Concepts for ecosystems to meet fundamental materials R&D data needs will also be discussed.

**8:20 AM**
**Structuring the Genome: Fundamental Materials Databases**: *Greg Olson*[1]; [1]Northwestern University

The 2004 NRC ATT study identified the role of the established small business ICME supply chain and called for a national Materials Genome Initiative to expand its underlying fundamental database structure. Advances in ICME applications have clarified the requirements for an enhanced database hierarchy.

**8:40 AM**
**Tools to Support the Flow of Traceable Materials Information Needed by ICME**: *Will Marsden*[1]; Beth Cope[1]; [1]Granta

ICME depends upon the successful integration of computational tools, experimental tools, and digital data in a seamless flow of traceable information. This paper will present insights gained through many years of working with the Materials Data Management Consortium, a group of highly materials-oriented commercial and government organizations in multiple sectors (including aerospace, defense, energy, oil, and gas). These experiences have highlighted the range of data involved: inputs, metadata, and results for both experimental data and computer generated models. They have shown that the right software tools are needed to maintain, visualize, and analyze the data, and to fully integrate it with computer-aided design and analysis packages. Crucial to providing secure, traceable, and accurate integration is an information architecture with the flexibility to store and utilize the full range of materials information, and comply with standards for communication of data (for example, that being developed by the CEN SERES project). This paper will present several examples from

industry, such as the need to handle both in-process, high-temperature data and its use in process modeling and supply chain data transfer. This poses challenges of verification and validation, and how to handle (and calculate) uncertainty. This paper will discuss these challenges and look at how best practice materials data management can meet the goals of ICME—by drawing on the experiences of leading enterprises as they seek to optimize their use of materials information in this way.

**9:00 AM**

**Data Informatics for Phase-Based Property Data**: *Carelyn Campbell*[1]; Ursula Kattner[1]; Alden Dima[1]; Doug Foxvog[1]; Philippe Dessauw[1]; Pierre Savonitto[1]; [1]National Institute of Standards and Technology

Current material property databases focus on either the engineering properties of commercial materials or on first principle results of selected material classes. The availability of phase-based property databases is limited, although these data are often essential for designing new materials. This work focuses on the development of informatics tools for phased-based property data. Experimental and computational phase-based property data, which serve as the basis for CALPHAD assessments, are diverse and semi-structured. In addition, these data sets are often incomplete (i.e. essential metadata is missing). To accommodate these incomplete data sets and the diversity of the data requires extensible representations. The strategy for developing these representations includes defining universal identifiers for materials, phases and crystal structures; a working ontology for phase-based materials; data schemas for specific material properties; and informatics tools. Implementation of this strategy for tracer diffusion and interdiffusion data will be demonstrated

**9:20 AM**

**Consideration of Ecosystem for ICME**: *Weiju Ren*[1]; [1]Oak Ridge National Laboratory

As the Integrated Computational Materials Engineering (ICME) becomes a hot topic, computation, experimentation and digital database are identified as three major components that support its development. Efforts in these three areas are being actively made from various aspects to bring ICME to reality. However, many factors that would affect ICEM development still remain vague. This paper is an attempt to identify cyberinfrastructure conditions for establishing a knowledge-base centered ecosystem that would facilitate ICEM development. The discussion includes relationship among these three major components, subcomponents that are crucial for a health development, and challenges and requirements for establishing the ecosystem.

**9:40 AM Break**

**10:00 AM**

**Exploiting Prior Physical Insights via Bayesian Statistics to Develop Accurate Localization Relationships via the Materials Knowledge System**: *Tony Fast*[1]; [1]University of California Santa Barbara

Top-down structure-property and structure-processing linkages are typically extracted through either computationally demanding simulation or limited empirical information. Recently, a novel framework, called the Materials Knowledge System (MKS), has been developed to construct accurate, bi-directional linkages in hierarchical material systems that enable computationally efficient multiscale modeling and simulation. The MKS extends digital signal processing methods to calibrate nonlinear filters that connect an input signal (ie. the microstructure) to an output signal (ie. the salient localized response). The filters, or influence coefficients, capture knowledge of the physical interactions embedded in either the simulation or experiment. Currently, the MKS is limited to materials systems that contain an ample database of microstructure-response data to provide the information to calibrate the filters. To extend the breadth of the MKS, a Bayesian framework has been formulated to explicitly incorporate physical insight into the calibration procedure. This novel Bayesian framework enables the MKS by reducing the requirements on the calibration database which lessens the computational demands in the calibration of the coefficients and makes the approach amenable to material systems with sparse calibration databases. We demonstrate this technique on building top-down structure-processing relationships for grain coarsening and spinodal decomposition microstructure evolution and structure-property relationships of the elastic response of multi-phase composites.

**10:20 AM**

**Cross-Scale Cross-Domain Model Validation based on Generalized Hidden Markov Model and Generalized Interval Bayes' Rule**: *Yan Wang*[1]; David McDowell[1]; Aaron Tallman[1]; [1]Georgia Institute of Technology

Reliable simulation protocols supporting integrated computational materials engineering (ICME) requires uncertainty to be quantified. In general, two types of uncertainties are recognized. Aleatory uncertainty is inherent randomness, whereas epistemic uncertainty is due to lack of knowledge. Aleatory and epistemic uncertainties need to be differentiated in validating multiscale models, where measurement data for unconventionally very small or large systems are scarce, or vary greatly in forms and quality (i.e., sources of epistemic uncertainty). In this paper, a recently proposed generalized hidden Markov model (GHMM) is used for cross-scale and cross-domain information fusion under the two types of uncertainties. The dependency relationships among the observable and hidden state variables at multiple scales and physical domains are captured by generalized interval probability. The update of imprecise credence and model validation are based on a generalized interval Bayes' rule (GIBR).

**10:40 AM**

**On the Use of Neural Networks to Develop an Understanding of the Roles of Continuum, Microstructural, and Compositional Variables on the Fracture Toughness of a/ß-processed TIMETAL®6-4**: *Peter Collins*[1]; Santhosh Koduri[2]; Vikas Dixit[3]; Hamish Fraser[3]; [1]University of North Texas; [2]Intel Corporation; [3]Ohio State University

Neural networks have been trained to permit an interpolative prediction of the interrelationships between continuum, microstructural, and compositional variables and the fracture toughness of a/ß-processed TIMETAL®6-4 (nominal composition TIMETAL®6-4, in wt.%). The variables included as inputs to the networks are the local tensile properties (yield strength, reduction in area), the local stress state at the crack tip through an inclusion of a plain strain thickness factor, quantified microstructural features and alloy composition, specifically the levels of Al, V, O, and Fe. The networks have been used to perform virtual experiments to permit determination of the functional dependences of these variables on fracture toughness. The networks are based upon an inclusion of an estimation of the plane strain thickness which captures the in-plane component of the stress state of the crack tip (sz), and also have as outputs both K1C and KQ values. It has, therefore, been possible to begin to estimate the effect of sample thickness on KQ and explore the magnitude of the difference between a measured KQ and K1C value. These results have significant implications regarding the understanding of the effect of microstructure on toughness and the ultimate prediction of toughness properties. The results of the neural networks have indicated key microstructural features that directly influence the fracture toughness of a/ß-processed TIMETAL®6-4. The role of key microstructural features have been validated and understood with an integrated experimental research effort.

**11:00 AM**

**Application of Statistical and Machine Learning Techniques for Correlating Properties to Composition and Manufacturing Process of Steels**: *Parijat Deshpande*[1]; BP Gautham[1]; Ahmet Cecen[2]; Surya Kalidindi[2]; Ankit Agrawal[3]; Alok Choudhary[3]; [1]Tata Consultancy Services; [2]Drexel University; [3]Northwestern University

Material scientists and engineers have been seeking correlations between various properties of metals, especially steels, and their compositions, manufacturing processes and microstructures. Numerous approaches have been explored, including physics-based, data-driven scientific methods as well as heuristics. However, fatigue being an extreme value property, has only enjoyed a limited amount of success with a combination of physics based models augmented with empirical models. In this paper, we explore a systematic data driven approach employing various dimensionality reduction and regression methods applied to the National Institute of Material Science public domain material database to arrive at meta-models for fatigue strength and present a careful assessment of the residual errors in each method. The implicit interdependencies of the data-set have been mitigated by QR factorization or clustering the data-set (Gautham et. al, ICME 2011). Multivariate regression techniques catering to incomplete data-sets and including easily measurable material properties as input variables to arrive at the predicted fatigue strength values are explored in this paper. The application of machine learning techniques such as neural network based regression to address the inherent non-linearity aspects of the available data and the results are compared with the earlier analyses. Regression analysis results using a neural network trained by Levenberg-Marquardt back propagation are presented in this paper. This paper aims to apply a combination of statistical and machine learning techniques supplemented by physics based understanding of the processes and composition to arrive at robust correlations for fatigue properties of a broad range of steels.

**11:20 AM**

**The GeoDict Virtual Material Laboratory: Integrated Software for Material Analysis and Synthesis**: *Andreas Wiegmann*[1]; Jürgen Becker[1]; Erik Glatt[1]; Matthias Kabel[2]; Heiko Andrä[2]; [1]Math2Market GmbH; [2]Fraunhofer ITWM

The dependence of materials properties on material geometry is emerging as a key aspect in many current material optimization applications. From fiber orientation and strut-thickness of sponges to effective stiffness and permeability tensors, the effect of geometry on material property is omnipresent. The GeoDict Virtual Material Laboratory is a generic approach to integrate the analysis of existing materials and the synthesis of new materials. By basing the computation of material properties on 3d images, the ready availability of µCT images can be exploited as well as the relative ease of creating 3d images from analytic representations and surface triangulations. Several powerful concepts are available: a scripting language for parameters studies and optimization studies. A generic description language of analytic data, together with conversion algorithms to surface triangulations and segmented 3d images. A multitude of integrated tools to convert abstract descriptions such as fiber diameter distribution, fiber orientation distribution and solid volume fractions into concrete 3d images, so-called realizations, and last but not least a multitude of integrated tools to predict material properties based on the geometry and constituent material properties. The most innovative (at least fast and memory efficient) ones are the Fast-Fourier-Transform based algorithms for integral equations and partial differential equations to estimate or to compute precise bounds of effective conductivity, diffusivity and stiffness, for example the FeelMath solver technology. In contrast to traditional approaches, complete anisotropic material tensors are predicted. See www.geodict.com for more details.

## Process Optimization

Tuesday AM Room: Ballroom D
July 9, 2013 Location: Salt Lake Marriott Downtown at City Creek

*Session Chair:* Peter Gumbsch, Fraunhofer Institute for Mechanics of Materials

**8:20 AM**

**Multi-scale, Multi-physics Optimization Framework for Additively Manufactured Structural Components**: *Tahany El-Wardany*[1]; Mathew Lynch[1]; Wenjiong Gu[1]; Arthur Hsu[1]; Michael Klecka[1]; Aaron Nardi[1]; Daniel Viens[1]; [1]United Technologies Research Center

This paper proposes an optimization framework that enables the integration of multi-scale/multi-physics simulation codes to perform structural optimization design. The developed framework first utilized topology optimization approaches for conceptual design, in which the component stiffness was maximized subject to constrained weight. A new design concept was determined with the topology optimization approach, followed by further shape optimization of the different component features based on design requirements (fatigue life and geometry). Cold Spray was selected as the additive manufacturing process and its manufacturing rules and constraints were identified and included in the optimization scheme. The subsequent optimization problem focused on stress-life fatigue analysis. Functionally graded materials were also explored through shape optimization techniques to further improve the design. During all optimization processing, the part geometry was morphed within limits of the additive manufacturing process selected to fabricate the part. The component weight was reduced by 25% while stresses were reduced by 3X, while the rigidity was improved up to 37% in comparison to the original design. All the programs were implemented using Altair OptiStruct, Altair HyperStudy, Abaqus, and in-house aerodynamic loading code. Finally, the optimized design was produced by the cold spray method using 410 stainless steel as the base material. A multiple splat impact model for cold spray was developed in LS-DYNA to define the optimum process parameters that can be used to eliminate processing defects and optimize particle/particle and particle/substrate bonding and resulting material properties.

**8:40 AM**

**Optimal Process Control through Feature-Based State Tracking along Process Chains**: *Melanie Senn*[1]; Norbert Link[1]; Peter Gumbsch[2]; [1]Karlsruhe University of Applied Sciences; [2]Fraunhofer Institute for Mechanics of Materials

The optimal control of linked individual manufacturing processes serves as a basis for the optimization of an entire process chain. The optimal control of a single process thereby aims at process parameters that achieve the optimal result with least effort while accepting and handling uncertainty. In contrast to classical control which is implemented by tracking a predefined optimal path in state space, the optimal path is here defined on the current state considering future uncertainties. This requires a description of the process which includes a representation of the state of the processed material. Only few observable quantities can usually be measured from which the state has to be reconstructed by real-time capable and robust observer models. This "state tracking" is performed by a mapping of the measured quantities on the state variables. This mapping is found by nonlinear regression based on statistical learning. The mapping also includes a dimension reduction to lower the complexity of the multi-stage optimization problem which is solved approximately online. This proposed generic process model provides a universal description that can be adapted to specific data from simulations or experiments. We have shown the feasibility of the generic approach by the application to a deep drawing process in which the state is described in terms of the local flow stresses in a workpiece of DC04 steel. The control concept developed here

can be extended to the optimization of entire process chains.

**9:00 AM**

**Leveraging ICME for Industrial Applications: Prospects, Progress & Challenges**: *Sanjay Sondhi*[1]; John Warren[2]; Shesh Srivatsa[2]; Jason Parolini[3]; [1]GE Global Research; [2]GE Aviation; [3]GE Power & Water

Realizing full potential of ICME for industrial applications requires not only robust materials modeling capabilities, but also multiple additional enablers. A starting point is to link materials models and relevant statistical methods into a Tool that can (a) examine the effect of material and processing variability, and (b) carry out sensitivity analysis to identify the most critical material/process parameters. Another key step is to develop the requisite hardware/software infrastructure that allows a diverse set of end users to access a combination of in-house and commercially available Tools/Software/Data. This talk will share our experiences of implementing the same at GE. Examples will be provided of materials modeling efforts that span multiple length-scales, and leverage a wide range of modeling approaches. In some cases, the models are stitched-together, and share information in a seamless fashion; while in others the information is passed discretely. The eventual emphasis is on predicting the microstructure and resulting properties of engineering alloys, based on alloy chemistry and processing conditions.

**9:20 AM**

**Application of ICME Methods for the Development of Rapid Manufacturing Technologies**: *Tobias Maiwald-Immer*[1]; Thomas Goehler[1]; Andreas Fischersworring-Bunk[1]; Carolin Körner[2]; [1]MTU Aero Engines GmbH; [2]University Erlangen-Nürnberg

Rapid manufacturing technologies are lately gaining interest as alternative manufacturing method. Due to the large parameter sets applicable in these manufacturing methods and their impact on achievable material properties and quality, support of the manufacturing process development by the use of simulation is highly attractive. This is specially true for aerospace applications with their high quality demand and controlled scatter in the resulting material properties. The applicable simulation techniques to these manufacturing methods are manifold, the paper will focus on the melt pool simulation for an SLM (selective laser melting) process which was originally developed for EBM (electron beam melting). It will be discussed in the overall context of a multi-scale simulation within a virtual process chain.

**9:40 AM Break**

**10:00 AM**

**Introduction of Materials Modelling into Processing Simulation**: *Zhanli Guo*[1]; Gary Huang[2]; Richard Turner[3]; Alisson da Silva[4]; Nigel Saunders[1]; Hendrik Schafstall[2]; Jean-Philippe Schille[1]; [1]Sente Software Ltd.; [2]Simufact Engineering GmbH; [3]University of Birmingham; [4]Federal University of Minas Gerais

Computer-aided engineering (CAE) simulation tools are increasingly being used in industry to speed up processing design and manufacturing. However such simulation is not yet completely "virtual", in that its validity is entirely dependent on the availability of appropriate material properties as input, which at present rely heavily on experimental measurements. The introduction of materials modelling into processing simulation has become popular in recent years, whereas the fundamental technical challenge has been the development of material models so as to calculate the material data that are essential for CAE simulation. This paper reviews the development of material models on solid phase transformation kinetics, strengthening mechanisms, microstructure-property relationships and deformation mechanics, via which many of the material properties required in CAE simulation can now be calculated, such as TTT/CCT diagrams, temperature dependent physical and thermophysical properties, and temperature and strain rate dependent mechanical properties (strength and flow stress curves). The development and assessment of such models, together with their application in CAE simulation, has successfully bridged the gap between nanoscale information and macroscale mechanical behaviour using meso- and micro-mechanical theoretical analysis. The calculated material data can now be easily transferred to many commercial CAE simulation tools. Some case studies are presented here to demonstrate the application of such data in the simulation of hot forming, welding and heat treatments using simulation packages such as SIMUFACT®, FORGE®, and DEFORM®. Keywords: CAE simulation, materials modelling, welding, hot forming, heat treatments.

**10:20 AM**

**An Evolutionary Approach to the Design of Transformation Induced Plasticity (TRIP)-Aided Steels**: Shengyen Li[1]; *Raymundo Arroyave*[1]; Chung Wang[1]; Ruixian Zhu[1]; Pedro Rivera-Diaz-del-Castillo[2]; Ibrahim Karaman[1]; [1]Texas A & M University; [2]University of Cambridge

Transformation-Induced Plasticity (TRIP)-assisted steels are good candidates for the next generation high strength automotive structural materials due to their high strength and relatively high ductility enhanced through strain-induced martensitic transformation of retained austenite. TRIP steels consist of multi-phase microstructures (ferrite, bainite, martensite and retained austenite), whose properties are greatly affected by their phase constitution, which in turn can be controlled through complex heat treatment schedules. In this work, we first present recently developed thermodynamic and kinetic models to predict the phase constitution of low-alloy TRIP steels as a function of heat treatment parameters. The models consider the partitionless nature of the bainitic transformation, the heterogeneous distribution of carbon as it is rejected from the bainitic ferrite into the remaining austenite and the stabilization of retained austenite against martensitic transformation due to carbon enrichment. The models are validated through detailed experimental work. The mechanical properties of the resulting multi-phase microstructure are investigated through strain hardening models taking into account the irreversible thermodynamics of dislocation generation (Rivera) and Mecking-Kocks-type models. The models (fitted to experiments) account for the strain-induced transformation of austenite (Olson-Cohen). The models for phase constitution and mechanical performance are then incorporated into a Genetic Algorithm optimization tool that optimizes strength and ductility of the microstructure as a function of heat treatment temperatures and alloy compositions. The model is tested against a low alloy TRIP steel with nominal composition Fe-0.32C-1.42Mn-1.56Si and is then applied for the development of a new class of TRIP steels with Fe-C-Mn-Si-Al-Cu as their major constituents.

**10:40 AM**

**Analytical Modeling and Performance Prediction of Remanufactured Gearbox Components**: *Raja Pulikollu*[1]; Nathan Bolander[1]; Sandeep Vijayakar[2]; Matthew Spies[3]; [1]Sentient Science Corporation; [2]Advanced Numerical Solutions LLC; [3]US Army Research Development and Engineering Command

Gearbox components operate in extreme environments, often leading to premature removal or overhaul. Though worn or damaged, these components still have the ability to function given the appropriate remanufacturing processes are deployed. Doing so reduces a significant amount of resources (time, materials, energy, manpower) otherwise required to produce a replacement part. Unfortunately, current design and analysis approaches require extensive testing and evaluation to validate the effectiveness and safety of a component that has been used in the field then processed outside of original OEM specification. To test all possible combination of component coupled with various levels of potential damage repaired through various options of processing would be an expensive and time consuming feat, thus prohibiting a broad deployment of remanufacturing processes across industry. However, such evaluation and validation can occur through Integrated Computational Materials Engineering (ICME) modeling and simulation. Sentient developed a microstructure-based component life prediction (CLP) tool to quantify and assist gearbox components remanufacturing process. This was achieved by modeling the material manufacturing process-microstructure-property relationship. The CLP tool assists in remanufacturing of high value, high demand rotorcraft, automotive and wind turbine gears. This paper will summarize the CLP models development, and validation efforts by comparing the simulation results with rotorcraft spiral bevel gear physical test data. CLP analyzes gear components and systems for safety, longevity, reliability and cost by predicting (a) new gear performance, and optimal time-to-remanufacture and (b) qualification of used gears for remanufacturing process.

**11:00 AM**

**A Mechanism-based Hierarchical Model Validated by Experimental Data**: *Dongsheng Li*[1]; Hussein Zbib[1]; Xin Sun[1]; Mohammad Khaleel[1]; [1]Pacific Northwest National Laboratory

An indispensible component of ICME is a predictive model on properties and structures evolution during mechanical deformation. We have developed a framework bridging molecular dynamics (MD), discrete dislocation dynamics (DDD), continuum dislocation dynamics (CDD), crystal plasticity (CP) and finite element method (FEM). One bright point in this framework is newly developed CDD with a novel constitutive law based on dislocation density evolution mechanisms. The dislocation density evolution law in this model is mechanism-based, with parameters measured from experiments or simulated with lower-length scale models, not an empirical law with parameters back-fitted from the flow curves. Applied on single crystal irons, this model was validated by experimental data. Comparing with traditional single crystal constitutive models with a Hutchinson-type hardening law and a dislocation-based hardening law, CDD model demonstrated higher fidelity. The traditional Hutchinson type hardening laws and other constitutive laws based on a Kock formulated dislocation density evolution law will only succeed in a limited number of loading directions. The main advantage of CDD is the novel physics-based dislocation density evolution laws in describing the meso-scale microstructure evolution. Another advantage of CDD is on cross-slip, important when loading conditions activate only one primary slip system. In addition to the dislocation hardening, CDD also takes into consideration dislocation defect interactions. Irradiation hardening of single crystal irons was simulated in this study with validation from experimental results. Further development will focus on integration of this framework into design tools to optimize processing and cut cost for development of advanced materials.

## Materials Data and Tools

Tuesday PM Room: Ballroom D&E
July 9, 2013 Location: Salt Lake Marriott Downtown at City Creek

*Session Chair:* Peter Lee, University of Manchester

**2:00 PM Introductory Comments:** Peter Gumbsch, Fraunhofer Institute for Mechanics of Materials

**2:05 PM Invited**

**Nanostructuring 1 Billion Tons: Integrating Multiscale Models, High-resolution Characterization and Combinatorial Synthesis for Designing Metallic Alloys**: *Dierk Raabe*[1]; M. Friak[1]; T. Hickel[1]; J. Millan[1]; S. Sandlöbes[1]; D. Ponge[1]; H. Springer[1]; I. Gutierrez[1]; P. Choi[1]; F. Roters[1]; D. Steinmetz[1]; S. Zaefferer[1]; J. Neugebauer[1]; [1]Max-Planck-Institut

Despite the existence of several thousand types of metallic alloys for structural applications more specific and well-tailored novel materials with superior properties are required for applications in the fields of industrial manufacturing, mobility, energy conversion, infrastructure, health, and safety. While properties of novel complex metallic multiphase materials can typically be to some extent successfully be developed and optimized with respect to desired properties by well-educated try-and-error methods through combinations of beneficial constitution and lattice defects, ab initio modeling techniques as well as an atomistic understanding of alloying enormously accelerate and guide this development process and render it into a more predictive and knowledge-based approach. Within the realm of ab initio electronic-structure theory, quantum-mechanical methods allow the generation of spin-dependent structural models of crystalline phases, the calculation of enthalpies, and the calculation of other measures, such as the stacking-fault energy and other lattice defects, as a function of temperature. These theoretical methods – together with atomic scale characterization (atom probe tomography, electron microscopy) and advanced combinatorial metallurgical synthesis - enable a novel methodological approach to metallic alloy design, as their results can be integrated into defect-density based continuum FE or FFT models to solve boundary value problems of complex microstructures. The talk presents this novel strategy of multiscale simulation and joint experimental structure analysis for exemplary types of structural materials, namely, ultra high strength steels.

**2:35 PM Invited**

**Microstructure Informatics for Mining Structure-Property-Processing Linkages from Large Datasets**: *Surya Kalidindi*[1]; [1]Drexel University

Materials with enhanced performance characteristics have served as critical enablers for the successful development of advanced technologies throughout human history, and have contributed immensely to the prosperity and well-being of various nations. Although the core connections between the material's internal structure (i.e. microstructure), its evolution through various manufacturing processes, and its macroscale properties (or performance characteristics) in service are widely acknowledged to exist, establishing this fundamental knowledge base has proven effort-intensive, slow, and very expensive for a number of candidate material systems being explored for advanced technology applications. It is anticipated that the multi-functional performance characteristics of a material are likely to be controlled by a relatively small number of salient features in its microstructure. However, cost-effective validated protocols do not yet exist for fast identification of these salient features and establishment of the desired core knowledge needed for the accelerated design, manufacture and deployment of new materials in advanced technologies. The main impediment arises from lack of a broadly accepted framework for a rigorous quantification of the material's microstructure, and objective (automated) identification of the salient features in the microstructure that control the properties of interest. Microstructure Informatics focuses on the development of data science algorithms and computationally efficient

protocols capable of mining the essential linkages in large microstructure datasets (both experimental and modeling), and building robust knowledge systems that can be readily accessed, searched, and shared by the broader community. Given the nature of the challenges faced in the design and manufacture of new advanced, this new emerging interdisciplinary field is ideally positioned to produce a major transformation in the current practices used by materials scientists and engineers. The novel data science tools produced by this emerging field promise to significantly accelerate the design and development of new advanced materials through their increased efficacy in gleaning and blending the disparate knowledge and insights hidden in "big data" gathered from multiple sources (including both experiments and simulations). This paper outlines a specific strategy (i.e. workflow) for data science enabled development of the materials genome and illustrates key components of the proposed overall strategy with examples.

**3:05 PM Invited**

**Big Data: A NIST Perspective**: *Mary Brady*[1]; Alden Dima[1]; [1]National Institute of Standards and Technology

The notion of big data is transforming scientific research by enabling data-driven discovery which automatically extracts new knowledge using techniques such as data mining, machine learning, and visualization. It is being enabled by the advent of multicore computing, parallel and concurrent software, and virtualization and new database and server architectures. These new technologies are being made accessible to the researcher via such innovations such as cloud computing which provides on-demand access to a shared pool of configurable resources and low-cost GPUs which promise massively parallel processing. Materials research, with its complex interrelated multi-scale data, is likely to benefit from multiple aspects of the big data paradigm. This talk will survey the impact of big data on scientific research from a NIST perspective.

**3:35 PM Break**

**3:45 PM Panel Discussion: Building a Materials Data Infrastructure for ICME**

## Poster Session II: ICME Applications

Tuesday PM Room: Ballroom AB&C
July 9, 2013 Location: Salt Lake Marriott Downtown at City Creek

**PII-35: A Computational and Experimental Study of the Vapor Deposition of Thermal Barrier Coatings onto Doublet Turbine Guide Vanes**: *Theron Rodgers*[1]; Hengbei Zhao[1]; Haydn Wadley[1]; [1]University of Virginia

Thermal barrier coatings deposited by physical vapor deposition are essential to the performance of modern aeroturbines. The coatings are deposited on complex-shaped components in the hot section of turbines to significantly increase the maximum allowable temperature. Current vapor deposition techniques require a direct line-of-sight to the substrate surface, which can require complicated movements during deposition and prevent deposition in channels between two surfaces. A recently developed directed vapor deposition technique uses a carrier gas to enable deposition onto non-line-of-sight substrate regions. A collection of computational tools has been utilized to simulate the ability of the directed vapor process to deposit uniform coatings on a doublet guide vane substrate. The computational tools include a direct simulation Monte Carlo code to model the rarefied gas environment in the deposition chamber, and a kinetic Monte Carlo code to simulate the microstructural development of the coating. The KMC code uses the substrate surface flux results of the DSMC routine to simulate the microstructural assembly of the coating. These results are stored in a database which is queried by a combinatorial optimization routine to determine the optimal processing conditions. The simulated optimal deposition conditions are then verified with experimental depositions.

**PII-36: A Computational Framework for Integrated Process Design for High Performance Parts**: *Rajiv Shivpuri*[1]; Kuldeep Agarwal[2]; [1]Ohio State University; [2]Minnesota State University

High performance parts such as aeroengine disks, transmission gears and bearings are manufactured in a sequence of processing steps starting from solidification processing, and followed by deformation processing, heat treatment and finish processing. The fatigue and failure performance of these parts are often governed by material and surface state, applied load and residual stress state, and the geometric design. Uncertainties in material structural including phase variabilities, inclusions, defects and anomalies, play a major role in the performance uncertainties and catastrophic failures. This poster will present a computational framework that enables integration of material and its processing history into the design activities. This computational framework will include integration of deterministic process models, knowledge discovery through data mining, and the use of statistics of extremes. The integration of process models with design framework is achieved through model decomposition based on the Bayesian probabilistic formulation. Efficacy of this approach will be demonstrated through application to selected manufactured parts.

**PII-37: A Continuum Model for the Growth of Anodic Alumina Films**: *Stephen DeWitt*[1]; Katsuyo Thornton[1]; [1]University of Michigan - Ann Arbor

Anodization is a technologically important technique for growing oxide films on metallic substrates. These oxide films have a wide range of applications including nano-templates, capacitors, solar cells, batteries, biomedical devices, sensors, and anti-corrosion finishes, and can either be nanostructured (e.g., nanoporous) or compact. The mechanisms underlying anodic growth are not yet fully understood. To provide improved understanding of these growth mechanisms, we present a new continuum model and one-dimensional simulations for anodic film growth incorporating high-field ionic conduction, Butler-Volmer reaction kinetics, and space charge within the film. We discuss the strategies used to validate the model using experimental data for the average electric field, the Al3+ ejection current, the embedded surface charge, and the equilibrium pore-base thickness. We also discuss the design of new experiments to provide missing information on key parameters and further validation of the model. Finally, we discuss the extension of the model into multiple dimensions for simulations of anodic nanopore growth and self-organization.

**PII-38: A Large Strain Visoplastic Self-consistent Model with Dynamic Recrystallization Behavior Considered for FCC Polycrystalline Materials at Elevated Temperature**: *Xiaohui Fan*[1]; Mei Li[2]; Dayong Li[1]; Shaorui Zhang[1]; Yinghong Peng[1]; [1]Shanghai Jiao Tong University; [2]Ford Motor Company

A constitutive model considering dynamic recrystallization(DRX) behavior of FFC polycrystalline aggregates at elevated temperature is developed. The crystal plasticity model coupled with DRX model is used to predict texture evolution, yield strength, and volume fraction and average grain size of DRX during uniaxial compression large deformation of homogenized AA 6061 casting. We compare predictions with and without DRX description and found that the latter one can give a better representation of experimental texture and strain stress curves.

**PII-39: A Microstructure-strength Calculation Model for Predicting Tensile Strength of AlSiMg Alloy Castings**: *Shi Yufeng*[1]; Liu Baicheng[1]; Xu Qingyan[1]; Wu Qinfang[2]; Yang Hongwei[2]; [1]Tsinghua University; [2]Mingzhi Technology Co., Ltd.

The mechanical properties of $AlSi_7Mg$ alloys are known to be improved by heat treatment. By OM analyses and tension test, the effects of secondary dendrite arm spacing (SDAS) on tensile properties of $AlSi_7Mg$ alloys were investigated by using step-shaped castings. Finally, a calculation model of SDAS-tensile properties was developed. Based on the temperature field simulation by FT-STAR, an MCA model was used for simulating the dendrite morphology and SDAS values of $AlSi_7Mg$ alloy castings. Using the SDAS values and the calculation model, ultimate tensile strength and elongation would be predicted of $AlSi_7Mg$ alloy valve body, which compared well with the experimental data and meet the requirement.

**PII-40: A New Multi-scale Modeling Approach for Characterizing the Mechanical Properties of CNT Composites**: *Saeed Herasati*[1]; Liangchi Zhang[1]; [1]The University of New South Wales

This paper establishes a new multi-scale modeling approach to characterize the mechanical properties of nano-composites. The integration of the atomistic-macroscopic mechanical properties was realized by using a nano representative volume element (NRVE) containing both the matrix and the nano reinforcement phase such as nano-fibres and carbon nano-tubes (CNTs) . The properties of the NRVE, was obtained by employing molecular dynamics (MD) and molecular mechanics (MM) while COMPASS force field was in practice and the Material Studio software was employed for atomistic simulation. The introduction of the NRVE concept enables the realistic modeling of the contributions of wavy nano-fibres or CNTs to the macroscopic composite properties using a commercially available finite element code. The applicability and flexibility of this new approach was exemplified by an investigation into the property characterization of a nano-composite of Polyvinylchloride (PVC) matrix reinforced by single-walled carbon nanotubes. From nanoscale simulation , it was concluded that the effect of nano-inclusion on the adjacent matrix and the vdW force effect have major impact on the overall properties of nanocomposite which is covered by NRVE furthermore, the new established approach can be applied to a wide range of advanced composites containing nano-scale reinforcements with complex morphology where multi-scale interactions would play an important role.

**PII-41: CANCELLED: An Experimental and Modeling Investigation on High-Rate Formability of Aluminum**: *Aashish Rohatgi*[1]; Richard Davies[1]; Ayoub Soulami[1]; Elizabeth Stephens[1]; Mark Smith[1]; Gary Vanarsdale[1]; [1]Pacific Northwest National Laboratory

This presentation will describe the integrated experimental and modeling effort at PNNL to enable room-temperature forming of aluminum alloys by taking advantage of enhanced formability associated with high-strain-rate forming processes. The strain-rates in such forming processes are highly variable over the event duration and the formability, failure modes and constitutive relations of most metallic materials can be dramatically different under different strain-rate regimes. Hence, the ability to develop validated models of the forming process is extremely important to enable its industrial implementation. However, validated models of high-rate forming processes are typically not found in the literature on account of experimental difficulties in determining the deformation history during such short duration events. In this work, AA5182-O Al alloy sheets were deformed under biaxial stretching and in near plane-strain conditions, at strain-rates typically exceeding 1000 /s, using the electrohydraulic forming (EHF) technique. Sheet deformation was modeled in Abaqus and validated with experimentally determined deformation data. Tensile tests under quasi-static and dynamic strain-rates were performed to determine the strain-rate sensitivity of AA5182 as a function of strain-rate. This work will use the M-K method and parametrically investigate and predict the influence of strain-rate on the formability of AA5182.

**PII-42: An ICME Approach to Solute Strengthening of Aluminum and Magnesium Alloys**: Louis Hector Jr[1]; Gerard Leyson[2]; William Curtin[3]; *David Howe*[4]; [1]General Motors; [2]Brown University; [3]Ecole Polytechnique Federal de Lausanne; [4]TMS

Integrated computational materials engineering (ICME) is fueling a global renaissance in metallurgical research and the design of new alloys with enhanced properties. As materials that are commonly labeled as "traditional," both ferrous and non-ferrous alloys are now being re-examined with exciting new computational and experimental tools that are part of developing ICME frameworks. In this talk, we shall examine one such framework within which a quantitative, parameter-free theory of solute strengthening of aluminum and magnesium alloys is developed. Expressions for the alloy yield strength as a function of temperature and strain rate are informed with solute-dislocation energetics computed with state-of-the-art first principles density functional theory (DFT) and a lattice Green's function method. For Al alloys, strengthening due to Mg, Cr, Cu, and Si solutes is quantified; for Mg, focus is on strengthening of basal flow stress in Mg-Al alloys. Model predictions compare favorably with experimental data. Key differences in strengthening due to the size of the equilibrium dislocation core structures will be emphasized. The models are readily extended to other solute chemistries and dislocation types. A brief overview of a new ICME project on third generation advanced high strength steels funded by the U.S. Department of Energy will be provided (http://energy.gov/articles/energy-department-investments-develop-lighter-stronger-materials-greater-vehicle-fuel).

**PII-43: An Integrated Approach to Determine Complex Phenomenological Equations in Metallic Systems**: *Peter Collins*[1]; Iman Ghamarian[1]; [1]University of North Texas

A novel approach has been developed that seeks to move beyond the interpolative predictive capabilities of artificial neural networks. Artificial neural networks are a powerful tool to understand complex interdependencies that may exist among various input features (e.g., composition and microstructure) and an output (e.g., yield strength). These models have been shown to be successful at predicting properties in Ti-based alloys. However, the form of the equations commonly relies upon very flexible mathematical equations such as the hyperbolic tangent function. Such functions are quite different than the phenomenological equations that often appear when considering the physical metallurgy of a system and strengthening mechanisms. We have developed an approach where genetic algorithms have been used in an integrated fashion with artificial neural networks and the Monte Carlo approach to help determine an optimized phenomenological equation for strength in multi-component, multi-phase engineering alloys. This approach can be readily extended to other material problems where the precise physics may be unknown, but for which there is a strong theoretical basis on which to postulate forms complex phenomenological equations for which the precise details are unknown. This is applied to alpha+beta processed Ti-6Al-4V material with intentional variations in microstructure and composition to predict the yield strength. Details of the phenomenological equation are rationalized, where possible, against the limited mechanistic details. This approach should help to reduce the amount of database development that is required in the future.

**PII-44: An Integrated Computational and Experimental Study for the Size Effect of the Cu Precipitation on the Mechanical Response of Microalloyed Steel**: *Shijin Zhao*[1]; Lijuan Hu[1]; [1]Shanghai University

The effect of size of nanoscale Cu precipitate on the mechanical response of microalloyed steel was investigated computationally and experimentally. A phenomenological constitutive description is adopted to build the computational crystal model. The material is envisaged as a composite; the Cu precipitate is modeled as a monocrystalline core surrounded with a lower yield stress and higher work hardening rate response. Both a quasi-isotropic and crystal plasticity approaches are used to simulate the matrix. The nanoscale precipitate is modeled as ellipsoidal inclusion with different Yound's modulus to matrix. Elastic

and plastic anisotropy are incorporated into this simulation. An implicit Lagrangian finite element formulation with von Mises plasticity or rate dependent crystal plasticity is used to study the nonuniform deformation and localized plastic flow. The computational predictions are compared with the experimentally determined mechanical response of HSLA-100 steel with average size of nanoscale precipitates of 2.02±1.89nm. The tendency of the calculated yield strength attributed to Cu precipitates is in good agreement with experimental result.

**PII-45: Computational Modeling of Electrochemical Charge/ Discharge Behavior of Li-ion Cells**: *Madhu Jagannathan*[1]; K. S. Ravi Chandran[1]; [1]University of Utah

Modeling of charge/discharge behavior of Li-ion cells, in particular the electrochemical insertion and de-insertion of $Li^+$ is challenging because of the complexity of the ion transport and phase transformations corresponding to intercalation/deintercalation. Mesoscopically, this requires analytical solutions of diffusion that incorporate moving phase boundaries due to phase transitions. Here, we present a computational scheme, using which one can predict the charge/discharge behavior of Li-ion cells. The computational scheme uses analytical diffusion solutions for each electrode, which include moving phase boundaries. The migration and diffusion of $Li^+$ ions within the electrolyte are modeled using the Nernst-Planck equation. Butler-Volmer kinetics is used to calculate the charge transfer overpotentials at the two electrode/electrolyte interfaces. A comparison of the simulation results with experimental data is presented. The computational scheme is more direct, intuitive and can be adopted to simulate the behavior of Li-ion batteries.

**PII-46: Design Optimization of Transmission of $Si/SiO_2$ and $Ge/SiO_2$ Multilayer Coatings**: *Khurram Iqbal*[1]; Jianjun Sha[1]; Asghari Maqsood[2]; [1]Dalian University of Technology; [2]National University of Sciences and Technology

Integrated computational materials engineering (ICME) is an emerging discipline that provides a wealth of information, breaks down the technological barriers and optimizes the experimental setups. The development of computational tools for materials engineering requires physical phenomena that must be captured and integrated with various materials-related disciplines and organization types. This integration discriminates between the materials development cycle and the product development cycle and reduces the length of the materials development cycle from 10 years to 2 years. TFCalc software was used for optical designing .This article includes some mathematical models such as the spectral distribution of $Si/SiO_2$ and $Ge/SiO_2$ coatings transmittance.

**PII-47: Ductility Prediction for Complex Magnesium Alloy Castings Using Quality Mapping**: *Jiang Zheng*[1]; Mei Li[1]; Joy Forsmark[1]; Jacob Zindel[1]; John Allison[1]; [1]Ford Motor Company

In this work, carefully controlled casting experiments were conducted and the mechanical properties were experimentally determined in different locations in complex magnesium casting. Each processing condition was simulated using the MAGMAsoft and the simulation results were determined from each location. Quality mapping (QM) was established to predict the mean ductility and statistic variation in AM60 Magnesium casting. The QM was validated using another vehicle component casting.

**PII-48: Electronic, Structural and Elastic Properties of (V,Nb)Cx**: *Krista Limmer*[1]; Julia Medvedeva[1]; [1]Missouri S&T

Carbide formation and stabilization in steels is of great interest due to its effect on the microstructure and properties of the Fe-based alloys. Achieving fine, homogeneously dispersed high strength carbide precipitates is one of the challenges required to meet the demands of the automotive industry for high strength lightweight steels. Carbide forming elements such as Ti, Nb, V, Cr, and Mo have been examined as possible additions. Vanadium has been of interest due to the increased solubility of VC in the iron matrix, compared with TiC and NbC. This allows for dissolution of the VC into the steel during heating and fine precipitation during cooling. The primary vanadium carbide of interest for steel applications, VC, has a cubic NaCl-type crystal structure. However, non-stoichiometric compositions VCy have been observed, where y has a wide range from 0.72 to 0.88. Within this range, two ordered compounds V8C7 and V6C5 exist. In this study a first-principles density functional approach is used to examine the formation and stability of the binary vanadium carbides with respect to the crystal structure by calculating their formation energies. We compare the local structures (atomic coordination, bond distances and angles) and the density of states in optimized geometries of the carbides. Further, the influence of alloying additions, such as niobium, on the carbide stabilization is also investigated. We determine the energetically preferable substitutional atom location in each carbide and study the impurity distribution as well as its role in the carbide formation energy and electronic structure.

**PII-49: Geometric Analysis of Casting Components**: *Quan Zhibin*[1]; Gao Zhiqiang[1]; Wang Qigui[2]; Sun Yunxia[1]; Chen Xin[1]; Wang Yucong[2]; [1]Southeast University, China; [2]General Motors Holdings LLC

Automated manufacturability analysis, aiming to considerate manufacturability aspects at initial stages of product design, is important for the designers in modern manufacturing industry to design manufacturable components. It mainly assists designers to economize the cost and time without compromising the quality and functional requirements of manufacturable parts. This paper deals with feature recognition for automated manufacturability analysis of new casting product. A new region growing method and an octree-based wall thickness computation approach are developed to extract manufacturing features (such as cylinder holes and wall thickness), from a CAD model which is represented by STL format.

**PII-50: Integrated Computational Materials Education Summer School**: *Larry Aagesen*[1]; Anton Van der Ven[1]; Jonathan Guyer[2]; Laura Bartolo[3]; Greg Olson[4]; John Allison[1]; Paul Mason[5]; Edwin Garcia[6]; Mark Asta[7]; Katsuyo Thornton[1]; [1]University of Michigan; [2]National Institute of Standards and Technology; [3]Kent State University; [4]Northwestern University; [5]Thermo-Calc Software; [6]Purdue University; [7]University of California Berkeley

ICME has emerged as a promising approach to the development of new materials for a variety of applications. An important component of growing the use of the ICME approach to materials development is engaging the next generation of scientists and engineers. To encourage the spread of computational methods used in ICME into the undergraduate Materials Science and Engineering curriculum, we developed the Integrated Computational Materials Education (ICMEd) Summer School, held at the University of Michigan in Ann Arbor, MI, in 2011 and 2012. This Summer School is a two-week program that includes a "crash course" on computational materials science and engineering techniques taught by experts in each area, as well as "modules" which target the introduction of computational techniques into core courses in the undergraduate MSE curriculum, such as thermodynamics, kinetics, mechanics, and physics of materials. Each module consists of a detailed explanation of the computational technique, review lecture tying the computational method to fundamental MSE concepts, a walk-through detailing how to use the software, and a problem set to apply the concepts. Participants are encouraged to use these modules at their home institutions. The Summer School will be held again beginning in summer 2014. A shortened version will be offered as a Short Course in conjunction with the ICME Congress. The application to participate is open to faculty, postdoctoral researchers, and graduate students from MSE departments in both the U.S. and abroad (financial assistance will available for participants from U.S. institutions).

**PII-51: Integrated Computational Model for Resistance Spot Welds in Auto-body Crashworthiness CAE: Process, Properties, and Performance**: *Lili Zheng*[1]; Yanli Wang[1]; Srdjan Simunovic[1]; Wei Zhang[1]; Zhili Feng[1]; [1]Oak Ridge National Laboratory

An integrated resistance spot weld process-properties-performances modeling approach is developed to characterize the multi-physical phenomenon during welding and the subsequent crash evaluation. The modeling framework begins with the process model that performs coupled electrical-thermal-mechanical computations to determine the temperature history and weld nugget growth based upon prescribed welding conditions. The microstructure-property model determines the microstructure and property gradients in resistance spot welds based on steel's composition and temperature history of the welding process. A detailed 3-D structural model taking into account of the local microstructure and property gradient in the weld region (predicted from the microstructure-property model) is used to reveal inherent failure features as well as to determine the failure parameters, based on the damage mechanics principles. Finally, a robust spot weld element (SWE) is formulated based on the knowledge gained in the detailed 3-D model for use in crashworthiness engineering and optimization of spot welded advanced high-strength steel auto-body structure components.

**PII-52: Integrated Realization of Engineered Materials and Products: A Foundational Problem**: Janet Allen[1]; Farrokh Mistree[1]; Jitesh Panchal[2]; *BP Gautham*[3]; Amarendra Singh[3]; Sreedhar Reddy[3]; Nagesh Kulkarni[3]; Prabhash Kumar[3]; [1]University of Oklahoma; [2]Purdue University; [3]TRDDC, Tata Consultancy Services

In the last several years, considerable ICME related research has been directed towards the study of multiscale materials design. However, relatively little effort has gone into the study of the integrated design of engineered materials and products. In this paper, we describe a foundational problem that is being used to validate and demonstrate the ICME construct and enable design approaches and a computational platform. The foundational problem involves the integrated design of steel and gears, traversing across the chain of steel making, mill production, component fabrication and performance testing tracking the evolution of the material during these processes and linking this to the mechanical design of the component. The design approaches are focused on addressing the following key challenges in the integrated design of products and materials: uncertainty management, complexity management, and holistic verification and validation. The management of uncertainty and complexity is critical to understanding the relation¬ship between computational costs and the value of the resulting information in the design decision making process.

**PII-53: Microstructure Mediated Design of Material and Product**: Ayan Sinha[1]; Janet Allen[2]; Jitesh Panchal[1]; *Farrokh Mistree*[3]; [1]Purdue University; [2]University of Oklahoma, Norman; [3]University of Oklahoma

In this paper, the construct of microstructure-mediated design is explored by framing a multiscale system with the appropriate aspects of the material microstructure, followed by multiscale material modeling, and then engineering the microstructure using the Inductive Design Exploration Method, to achieve the product specifications. As the microstructure represents the limiting interface between structure-property relations including system performance and process-structure relations, we have adopted the phrase microstructure mediated design. We illustrate the efficacy of this construct via the integrated design of a submersible and an Al-based matrix composite.

**PII-54: Modeling and Verification of Vacuum Carburizing Process for 20Cr$_2$Ni$_4$A Steel**: Shaopeng Wei[1]; Gang Wang[1]; Yiming Rong[1]; [1]Tsinghua University

Vacuum carburizing process has the advantage of more uniform diffusion layer, the shorter process time and little oxides. The optimum parameters for the process can be obtained and improved by using numerical simulation technology. In this paper, a vacuum carburizing model has been built and verified. Meantime complete tests on carburized samples of 20Cr2Ni4A steel had been conducted on microstructure, hardness profile, carbon content and surface retained austenite. The simulation results were in accord with the experimental measurements. This model can be used to improve the further practice.

**PII-55: Modelling the Process Chain of Cold Rolled Dual Phase Steel for Automotive Application**: *Ulrich Prahl*[1]; Ali Ramazani[1]; [1]RWTH Aachen University

Dual phase (DP) steels consorting of a dispersion of hard martensite particles in a ductile ferrite matrix belong to the class of modern advanced high strength steels for lightweight design in automotive applications. Typically, this steel concept undergoes a long process chain starting with cold rolled sheet, following with a multistep intercritical annealing including quenching plus hot dip coating, forming to a part and finally annealing of the formed and painted part. It is shown that all process steps might have an influence on the final properties of the part. Thus, the precise control of the microstructure evolution during full processing route is required for the achievement of essential mechanical properties. This project aims to develop a virtual process chain for the production of components out of cold rolled DP steel. The simulation chain starts with cold-rolled strip. During intercritical annealing process all relevant steps like recrystallization, austenite formation and grain growth, ferrite and martensite transformation including bainite fractions and quasi-tempering during hot dip coating and coiling are taken into account. Concerning the final mechanical properties transformation induced micro eigenstresses are described as well as strain partitioning on microscale during cold forming. Finally the bake hardening process is described and the strength increase is quantified following a microstructure based approach. This multi-scale and process-spanning approach enables the local properties in the part for varying composition and processing conditions. Thus, it can be used for the knowledge driven design and optimization of tailored material and process.

**PII-56: Multi-Objective Optimization of Wrought Magnesium Alloy Microstructure for Strength and Ductility**: *Bala Radhakrishnan*[1]; Sarma Gorti[1]; Srdjan Simunovic[1]; [1]Oak Ridge National Laboratory

The microstructural features that govern the mechanical properties of wrought magnesium alloys include grain size, crystallographic texture, and twinning. Several processes based on shear deformation have been developed that promote grain refinement, weakening of the basal texture, as well as the shift of the peak intensity away from the center of the basal pole figure - features that promote room temperature ductility in Mg alloys. At ORNL, we are currently exploring the concept of introducing nano-twins within sub-micron grains as a possible mechanism for simultaneously improving strength and ductility by exploiting a potential dislocation glide along the twin-matrix interface – a mechanism that was originally proposed for face-centered cubic materials. Specifically, we have developed an integrated modeling and optimization framework in order to identify the combinations of grain size, texture and twin spacing that can maximize strength-ductility combinations. A micromechanical model that relates microstructure to material strength is coupled with a failure model that relates ductility to a critical shear strain and a critical hydrostatic stress. The micro-mechanical model is combined with an optimization tool based on genetic algorithm or gradient descent method. A multi-objective optimization technique is used to explore the strength-ductility space in a systematic fashion and identify optimum combinations of the microstructural parameters that will simultaneously maximize the strength-ductility in the alloy. Research sponsored by the Laboratory Directed Research and Development program at Oak Ridge National Laboratory, managed by UT-Battelle, LLC, under contract DE-AC05-00OR22725 for the U.S. Department of Energy.

**PII-57: Multi-Scale Modeling of Ni/YSZ Fuel Cell Anode**: *Ji Hoon Kim*[1]; Wing Kam Liu[2]; Christopher Lee[2]; [1]Korea Institute of Materials Science; [2]Northwestern University

Performance and degradation of fuel cell components are discussed in a multi-scale framework in this paper. Electrochemical reactions in a

solid oxide fuel cell occur simultaneously as charge and gas pass through the anode, electrolyte, and cathode to produce electric power. Since fuel cells typically operate at high temperatures for long periods of time, performance degradation due to aging of the fuel cell materials should be examined. This phenomenon is treated in a multi-scale framework by considering how microstructure evolution affects the performance at the macro-scale. Mass and charge conservation equations and electrochemical kinetic equations are solved to predict the overall cell performance using the local properties calculated at the micro-scale. Separately, the microstructures assigned to the macroscopic integration points are evolved via the Cahn-Hilliard equation using an experimentally calibrated kinetic parameter. The effective properties of the evolving microstructure are obtained by homogenization and incorporated in the macro-scale calculation. The proposed model is applied to a solid oxide fuel cell system with a nickel/yttria stabilized zirconia (Ni/YSZ) cermet anode. Our model predicts performance degradation after extended hours of operation related to nickel particle coarsening and the resulting decrease in triple phase boundary (TPB) density of the anode material. The investigation of the microstructural effects on TPB density suggests that using Ni and YSZ particles of similar size may retard performance degradation due to anode aging.

**PII-58: Quantitative Characterization of Precipitate Microstructures for Use in ICME Models for Magnesium Alloys**: *Jiashi Miao*[1]; [1]University of Michigan

Magnesium alloys are becoming increasingly important for use in the transportation industry however current limitations in their capabilities require new alloys. Integrated computational materials engineering (ICME) is a powerful tool for designing new magnesium alloys or optimizing the processing techniques of magnesium alloys currently in industry application. Precipitation hardening is an important strengthening mechanisms for magnesium alloys, however our current predictive, quantitative understanding of alloying effects on precipitate evolution is limited. In this study, we study evolution of precipitate microstructures in the magnesium alloy AZ91 as a "model" material for development of a more comprehensive understanding of this important phenomenon. A combination of quantitative TEM, STEM and Atom Probe Tomographic characterization were used in conjunction with phase field and first-principles modeling (which are the focus of a companion paper). This talk focuses on the techniques required for quantifying morphology, 3D size and number density of precipitates in this alloy. Atomic structure of precipitates and interfacial structure between precipitates and magnesium matrix was characterized using high angle annular dark field-STEM method. The distribution of different alloying elements in precipitation microstructure was quantitatively determined using atom probe tomography. These experimental results have been used as critical inputs for an ICME tool developed for magnesium alloys. A physically based precipitation strengthening models was developed for this alloy to predict the effects of different heat treatment parameters on the yield strengthen of this alloy.

**PII-59: Study of Numerical Simulation on Quenching Distortion in a Steel Component with Internal Thread**: *ZhenGuo Nie*[1]; Gang Wang[1]; Yiming (Kevin) Rong[1]; [1]Tsinghua University

An steel component has a slight distortion in internal thread position when it undergoes a quenching process. But this small distortion affects assembly severely in the precision engineering. Using FEA software with its user subroutines, the position and contour of distortion which are confirmed by subsequent experimental measurement are simulated. And it also provides the improvements to machining and heat treatment process. Such suggestions improve the manufacturing process significantly.

**PII-60: The Finite Element Analysis Of Thermal Field and Stress Field in the Heavy Locomotive Wheels**: *ZhenGuo Nie*[1]; Wei Shi[1]; Gang Wang[1]; Yiming (Kevin) Rong[1]; [1]Tsinghua University

Decouple the thermal field and the stress field in HXD2 heavy locomotive wheels when it works in different working conditions, and then calculate the thermal field first. Secondly,stress and strain fields are calculated basing on the thermal field. In the different working conditions, curves of stress and strain changing with time are drawn respectively, and also the temperature rising curve in the treads as the train brakes. All the works will provide the calculation basis to assessment of fatigue performance and wear behavior.

**PII-61: The Microstructure and Micromechanical Properties of Zr-Cu-Fe-Al Bulk Metallic Glass Irradiated by High-energy $Ar^+$ Ion**: *Bin Yang*[1]; Wendong Luo[1]; Lu Yang[2]; Xitao Wang[1]; [1]University of Science and Technology Beijing; [2]Department of Metallurgical Engineering, The University of Utah

Plate-like $Zr_{61.5}Cu_{21.5}Fe_5Al_{12}$ specimens were irradiated by 300 keV $Ar^+$ ions to total fluences from 3\215 $10^{15}$ to 3\215 $10^{16}$ $cm^{-2}$. The reason why we select 300 keV $Ar^+$ ions irradiation is because it can attain the implantation depth of around 354 nm and considerable radiation damages calculated by using the Stopping and Range of Ions in Matter (SRIM) code, which meets nanoindentation experiments demand. XRD results showed that the alloy specimens still maintained amorphous structures. HRTEM and selected area diffraction results, however, showed that a nanocrystalline fcc phase was formed when irradiated to a fluence of 1\215 $10^{16}$ $cm^{-2}$. Moreover, lattice distortion defect was formed in the nanocrystals when the ion irradiation dose was increased up to 3\215 $10^{16}$ $cm^{-2}$. Differential scanning calorimetry analysis proved that the $T_g$ of the bulk metallic glass (BMG) decreases from 675 to 661 K with increasing $Ar^+$ ion irradiation dose up to 3\215 $10^{16}$ $cm^{-2}$. As a result, the supercooled liquid region is broadened up to 106 K. This indicates that $Ar^+$ ion irradiation is very effective in enlarging the supercooled liquid region of the BMG. Nanoindentation results showed further that the hardness and Young's modulus of the alloy increased with increasing ion irradiation doses. The improvement in the hardness of the alloy is due to the formation of nanocrystals, which causes the pinning of shear bands. The improvement in the elastic modulus is due to the nanostructured precipitates, which decrease the interatomic distance of the alloy.

**PII-62: The Study on the Induction Heating System: The Establishment of Analytical Model with Experimental Verification and the Phenomenological Study on the Process from Simulation Perspective**: *Tianxing Zhu*[1]; Feng Li[1]; Xuekun Li[1]; Yiming Rong[2]; [1]Tsinghua University; [2]Worcester Polytechnic Institute

Induction heating is frequently used in the metalworking industry to heat metals for hardening, soldering, brazing, tempering and annealing. But due to its complexity, the analytical model for the induction heating process is still under progress. Therefore, the need of using simulation to analyze the induction heating process could become very advantageous both in design and economic aspects. In this paper, an analytical model is established and verified by the experiments, including workpiece emissivity calibration. After the establishment of analytical model, phenomenological study on the effect of magnetic flux concentrator, current parameters were conducted. The FEM simulation helps to further understand the induction heating process, and to quantify the effect of input parameters. Therefore, it is possible to better optimize the process, and to develop new techniques.

**PII-63: Towards an Integrative Simulation of Microstructural Response to Case Hardening of Microalloyed Steels**: Patrick Fayek[1]; Thomas Petermann[1]; *Ulrich Prahl*[1]; [1]RWTH Aachen University

Case hardening is more efficient when the process is carried out at elevated temperature. The process is though limited by grain coarsening phenomena which occur when the state of precipitates in the material is not sufficient. The presented approach comprises the estimation of the precipitate volume and size dependent on chemical composition, temperature and previous processin steps. The microstructural response is subsequently estimated using the phase-field approach. Different microalloying concepts based on Al, Nb and Ti will be simulated. Simulation of the grain coarsening behavior in relation to the precipitate condition is needed for pre-evaluation of processing schemes and materials design. Time and temperature evolution of the precipitates have to be considered causing particle ripening and dissolution as a function of nonisothermal heat treatments. Thus, the simulation of precipitates evolution in correlation with grain size stability as a function of the scale process parameters has to be realized along the whole process chain including various annealing steps. To describe all the relevant steps along the process, various simulation programs have been linked. A virtual platform is used for the communication and exchange of the simulation results. The exchange is realized in a universal data format. Using the comparison of simulation and experimental results the simulation platform and simulation tools can be optimized.

**PII-64: Two Thermal Conductivity Analysis of the Fuel Cell Zirconia Electrolyte, Evaluating the Point of Inflection**: *Oleksandr Kyrpa*[1]; [1]Frantsevich Institute of Problems of Materials Science

A new method of analyzing the electrical conductivity of the electrolyte based on zirconium ceramics, for fuel cell, using two thermal approach. That allows to determine the point of inflection on the curves for assistance with electrical breakdown temperature range for a few areas. Determination of activation energy minimization over functional abnormalities. Determination of grain size distribution depending on the sintering temperature of samples using image Lab, imageJ. Inflection point uniquely determines the characteristics DKKK, Praxair, IPMS 10Sc1CeSZ electrolytes in not depending on the sintering temperature in the range 1250 -1550 degrees, so it can serve as a constant for meteriala and is an integral characteristic.

**PII-65: Validation of High Strength Cast Al-Zn-Cu-Mg Aluminum for Use in Manufacturing Process Design**: *Maria Diana David*[1]; Robin Foley[1]; John Griffin[1]; Charles Monroe[1]; [1]University of Alabama at Birmingham

The wrought 7xxx series aluminum alloys are some of the highest strength aluminum alloys. Historically, cast alloys with similar compositions have not been produced because their long solidification ranges decrease castability and the intermetallics that form during solidification reduce ductility. To develop cast Al-Zn-Mg-Cu alloys, an understanding of the intermetallic formation is needed. Six experimental Al-Zn-Mg-Cu alloys were cast under 1 MPa (10 atmospheres) of pressure. Zinc concentrations of 8 and 12wt% and Zn: Mg ratios of 1.5 and 5.5 were produced. Copper was held constant at about 0.9wt%. Thermal analysis, x-ray diffraction, and scanning electron microscopy (SEM) were used to determine the solidus, liquids and time at solidus, and to identify the amount, composition and crystal structure of the as-cast intermetallics in the alloys. Thermodynamic modeling, via a CALPHAD method, was also used to predict these parameters. SEM and x-ray diffraction traces revealed that the intermetallics in the alloys were η and T. The volume fraction of these phases increased with zinc content and decreased with Zn:Mg ratio. The results predicted by calculation showed excellent agreement with the identification and amount of phases present. Calculation also accurately predicted the composition of the T phase while there was greater difference between the predicted and measured composition of the T phase. A comparison between the calculated and measured liquidus and solidus and time at solidus showed that the values followed similar trends and the closest predictions were of the liquidus temperatures.

**PII-66: Virtual Prototyping of Lightweight Designs Made with Cold and Hot Formed Tailored Solutions**: *Harald Porzner*[1]; [1]ESI North America

Tailored cold and hot formed solutions are the key to the lightweight construction of the future. Only tailored solutions allow the combination of soft and hard zones for best possible crash performance and minimum weight. The safety cage of future vehicles might be for example completely designed with hot formed components. To achieve the desired properties, a heat treatment process is part of the hot forming process. This poses additional challenges to the Automotive Industry – only perfectly heat-treated parts will fulfill specifications. The heat treatment process is a function of many parameters, and depends strongly on the forming process itself. Virtual Prototyping makes sure that component manufacturing and assembly processes yield to the designed tolerances and crash performance. ESI GROUP aims at providing all necessary tools for virtual prototyping of lightweight constructions designed and assembled with tailored solutions, in particular hot forming. This paper outlines what is needed for realistic virtual prototyping, and what is the status of the simulation solution. Validated realistic engineering examples are used to illustrate the capabilities in the field of virtual die design, forming, quenching, cooling channel engineering, assembly and product performance.

## ICME Building Blocks: Opening Session

Wednesday AM Room: Ballroom D&E
July 10, 2013 Location: Salt Lake Marriott Downtown at City Creek

*Session Chair:* Tresa Pollock, University of California Santa Barbara

**8:00 AM Invited**
**The Role of First-principles Calculations in ICME Approaches**: *Chris Wolverton*[1]; [1]Northwestern University

In order to optimize alloy design and processing conditions to quickly achieve materials with suitable mechanical properties, researchers in many groups are working on ICME approaches: suites of predictive computational tools that span length scales from atomistic to macroscopic to describe alloy microstructure, precipitation, solidification, and ultimately, mechanical properties. The role of first-principles computations in these ICME methodologies will be described, as will the connection between these first-principles methods and other computational approaches such as phase-field microstructural evolu-tion models, computational thermodynamics or CALPHAD methods, and cluster expansion methods and kinetic Monte Carlo. Applications will be shown to prediction of precipitation, microstructure evolution, and ultimately yield strength during heat treatment.

**8:30 AM Invited**
**High-Throughput Experimental Tools for ICME**: *Ji-Cheng Zhao*[1]; [1]The Ohio State University

The ICME efforts require reliable thermodynamic, kinetic and materials property databases as input to models for designing new materials as well as for optimizing processing for property enhancement and uncertainty quantification. This talk will review state-of-the-art experimental tools for rapid collection of experimental data to establish composition-phase-structure-property relationships. Efective model validation experiments will also be discussed. The experimental data serve the purposes of: 1) providing essential data for reliable database establishment, 2) discovering unusual effects to challenge and improve models, and 3) validating model predictions in an efficient manner. Examples will be used to illustrate these points.

**9:00 AM Question and Answer Period**

**9:10 AM Break**

## ICME Building Blocks: Experimental Tools

Wednesday AM Room: Ballroom D
July 10, 2013 Location: Salt Lake Marriott Downtown at City Creek

*Session Chair:* Richard Fonda, Naval Research Laboratory

**9:30 AM**

**Experimental Advances for ICME**: *Richard Fonda*[1]; David Rowenhorst[1]; [1]Naval Research Laboratory

Integrated computational materials engineering (ICME) is a powerful methodology that can shorten the time required for implementation while improving the quality of the components. However, the ICME process is limited by the experimental data used to model the system. Characterization of component microstructures is usually performed in a manner that differs little from what was used many decades ago. Instead, it is particularly important for the ICME community, which relies on limited experimental input to train and then verify the models used in this methodology, to accurately represent the constituent microstructures in order to improve the fidelity of the modeling process. This presentation will discuss the advances needed to improve the acquisition, characterization, and statistical representation of experimental information, particularly microstructures, to improve the acquisition time and accuracy of the ICME process. The primary developments that need to be pursued are the computer-friendly acquisition of microstructural information, the automated identification of components within that microstructure, the quantification of those microstructural constituents, and the statistical description of the microstructures.

**9:50 AM**

**Quantitative Characterization of Precipitate Microstructures for Use in ICME Models for Magnesium Alloys**: *Jiashi Miao*[1]; Emmanuelle Marquis[1]; Mei Li[2]; John Allison[1]; [1]University of Michigan; [2]Ford Research Laboratory

Magnesium alloys are becoming increasingly important for use in the transportation industry, however current limitations in their capabilities require new alloys. Integrated computational materials engineering (ICME) is a powerful tool for designing new magnesium alloys or optimizing the processing techniques of magnesium alloys currently in industry application. Precipitation hardening is an important strengthening mechanism for magnesium alloys, however our current predictive, quantitative understanding of alloying effects on precipitate evolution is limited. In this study, we study evolution of precipitate microstructures in the magnesium alloy AZ91 as a "model" material for development of a more comprehensive understanding of this important phenomenon. A combination of quantitative TEM, STEM and Atom Probe Tomographic characterization were used in conjunction with phase field and first-principles modeling (which are the focus of a companion paper). This talk focuses on the techniques required for quantifying morphology, 3D size and number density of precipitates in this alloy. Atomic structure of precipitates and interfacial structure between precipitates and magnesium matrix was characterized using high angle annular dark field-STEM method. The distribution of different alloying elements in precipitation microstructure was quantitatively determined using atom probe tomography. These experimental results have been used as critical inputs for an ICME tool developed for magnesium alloys. A physically based precipitation strengthening models was developed for this alloy to predict the effects of different heat treatment parameters on the yield strengthen of this alloy.

**10:10 AM**

**Advanced Dilatometry and Calorimetry for the Validation of Materials Mechanical and Transformation Models**: *Michael Reich*[1]; Benjamin Mikereit[1]; Olaf Kessler[1]; Matthias Krawutschke[1]; Christoph Schick[1]; Jan Kalich[2]; [1]University of Rostock; [2]Dresden University of Technology

For reliable process simulations it is no longer sufficient to focus on single manufacturing steps, but it is necessary to include all steps from casting via forming and machining to heat treatment in a process chain simulation. Accurate numerical simulation requires accurate temperature dependent material models to predict mechanical properties, microstructural changes, residual stresses and distortion. Dilatometry and calorimetry are in situ methods to detect changes in mechanical properties resp. microstructure during heating or cooling of the material. If substantial volume fractions participate in microstructural transformation, dilatometry allows the characterization of these microstructure changes. For example non-equilibrium states during martensitic transformation and tempering of steels can be analysed in this way. Another advanced method is given by Differential Scanning Calorimetry. Due to the fact that microstructural transformation can be an exothermic or endothermic reaction, the heat flow could be used as a measure of transformed microstructure amount and temperature range of transformation. The use of these both complementary experimental methods allows a critical consideration of the established results and has been exemplarily shown for the design of a short time heat treatment of the martensitic, press hardening, automobile body steel 22MnB5.

**10:30 AM**

**Non-contact Methods for Determination of Thermodynamic and Thermophysical Properties of High-temperature Materials**: *Robert Hyers*[1]; Jan Rogers[2]; [1]University of Massachusetts; [2]NASA MSFC

Advanced experimental methods provide data on thermodynamic and thermophysical properties needed for ICME. These data can be used directly as input for higher-level models or for validation of low-level models. Non-contact methods such as electrostatic and electromagnetic levitation allow measurements on reactive materials without chemical contamination from a container, as well as allowing access to the undercooled and metastable states. An overview of experimental methods will be presented for measuring different properties including phase diagrams, transformation kinetics, density and thermal expansion, and specific heat.

**10:50 AM Break**

**11:10 AM**

**3D Image Based Modelling for Computational Materials Applications - Taking 3D Imaging beyond Visualisation**: Philippe Young[1]; *Simon Richards*[2]; [1]University of Exeter; [2]Simpleware Ltd.

There has been increasing interest in the generation of computational models from 3D imaging modalities such as CT, microCT, and Microscopy for Materials Research. However, most mesh generation techniques currently available have not been developed for meshing from 3D imaging data. The paper will focus on techniques specific to image-based mesh generation, and will present a number of real-life examples in computational materials engineering such as composites, foams, soils, and 'as built' parts. The authors have developed surface and volume reconstruction algorithms that work directly on the image data, taking into account partial volume effects and providing sub-voxel accuracy. The technique is also topology and volume preserving, avoiding loss or gain of volume, and generates multi-part meshes that consist of matching nodes and elements without gaps or overlaps. Moreover, different density zones can be introduced which reduce the overall number of elements throughout the model whilst increasing the mesh density around areas of greater interest. The generation of micro-architectures with specific porosities conforming to an existing domain is also possible. Control of the domain's mechanical properties is achieved using a re-iso-surfacing technique which sets density variations throughout the architecture. In addition, the concept of a relative density map to represent the desired relative densities in the micro-architecture where the minimum and maximum porosity values can be specified is introduced. Finally, a homogenisation algorithm has been implemented. This enhances the value of the information obtained at micro level, enabling it to be used for macro models on desktop computers.

**11:30 AM**

**The 3D X-ray Crystal Microscope: An Unprecedented Tool for ICME**: *Gene Ice*[1]; John Budai[1]; Eliot Specht[1]; Bennett Larson[1]; Judly Pang[1]; Rozaliya Barabash[1]; Wenjun Liu[2]; Jonathan Tischler[2]; [1]Oak Ridge National Laboratory; [2]Argonne National Laboratory

There is a long-standing debate over the length scales needed to understand the behavior of materials and the role of surfaces, defects, and inhomogeneities. Indeed the properties of most materials are ultimately determined by defects that are either introduced during processing or in-service, and defect density and distribution must be considered for high-fidelity integrated computational modeling and engineering. Scientists at ORNL together with partners at Argonne have developed a powerful 3D X-ray Crystal Microscope that can nondestructively characterize the local 3D crystal structure of polycrystalline materials with submicron resolution and with sensitivity to the elastic strain tensor and the local Nye tensor. This emerging tool provides unprecedented tests of materials models under different processing/environmental conditions and provides new insights into the impact of unpaired dislocations, elastic strain and surfaces and interfaces. The promise of the original 3D Microscope and the emergence of similar instruments at synchrotrons around the world will be discussed with respect to ICME.Research sponsored by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division. Research performed in part on Beamline 34-ID of the Advanced Photon Source, a DOE BES User Facility.

**11:50 AM**

**Model Validation for Microstructural Sensitivities Using High Energy Diffraction Microscopy**: Moono Rhee[1]; Joel Bernier[1]; Shui Li[1]; John Bingert[2]; Jonathan Lind[3]; Nathan Barton[1]; [1]Lawrence Livermore National Laboratory; [2]Los Alamos National Laboratory; [3]Carnegie Mellon University

We present results from a model validation effort that employs detailed non-destructive three-dimensional microstructure data obtained from X-ray based High Energy Diffraction Microscopy (HEDM) experiemnts. The emphasis is on validating models that capture microstructural sensitivities so that these models can then be employed in rapid certification procedures. By focusing validation efforts on models that connect directly to experimentally measurable features of the microstructure, we can then build confidence in use of the models for components prepared under different processing routes, with different chemical compositions and attendant impurity distributions, or subjected to different loading conditions. The computational model makes use of a crystal mechanics based constitutive model that includes porosity evolution. The formulation includes nucleation behavior that is fully integrated into a robust numerical procedure, enhancing capabilities for modeling small length scales at which nucleation site potency and volume fraction are more variable. Three-dimensional experimental data are available both pre-shot and post-shot from the same volume of impact-loaded copper. Crystal lattice orientation and porosity data are obtained, respectively, from near-field HEDM and tomography techniques. Starting from the as-measured initial microstructure, simulation results will be compared to post-shot experimental results as a function of modeling assumptions. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 (LLNL-ABS-596472).

**12:10 PM**

**Atom Probe Microscopy**: Anna Ceguerra[1]; *Simon Ringer*[1]; [1]The University of Sydney

A key requirement for the success of ICME approaches is access to real-world databases of materials microstructure and properties. Without this critical element, the development of new materials and structures using informatics will founder. A particularly challenging domain is that of the 3D atomic-level structure of real engineering materials. Here, atom probe microscopy (APM) is in an excellent position to contribute, because it provides 3D positional information as well as the chemical composition of each atom. Some solutions to challenges associated with managing, visualising and analysing data in the order of tens to hundreds of millions of atoms are discussed.

## ICME Building Blocks: First Principles and Atomistic Tools

Wednesday AM Room: Ballroom E
July 10, 2013 Location: Salt Lake Marriott Downtown at City Creek

*Session Chairs:* Katsuyo Thornton, University of Michigan; Mark Asta, University of California, Berkeley

**9:30 AM**

**Validation of Atomistic Models within an Integrated Computational Environment**: *Paul Saxe*[1]; Clive Freeman[1]; Erich Wimmer[2]; [1]Materials Design, Inc.; [2]Materials Design, S.A.R.L.

Atomistic simulations are the foundation of integrated computational materials engineering. First-principles methods employ no materials specific parameters and, in contrast to larger-scale simulations, provide systematic predictions across a wide range of different materials. Indeed, it is now evident that first-principles calculations of structural, elastic, electronic, and magnetic properties have attained a level of generality and reliability that allows their use in the systematic cross-checking and augmentation of experimental data. In this contribution we provide an overview of the capabilities of leading first-principles methods, their direct use in the computation of materials properties, and their role in parameterizing and validating the next levels of simulation based on classical descriptions of interatomic interactions. The main focus will be on systematic model validation at both the quantum mechanical and the quasi-classical levels of atomistic simulations. Examples will include a range of industrially relevant properties for metals, oxides, sulfides and polymeric materials. The final part of the talk will be devoted to an assessment of the impact of the increasing power of high-performance parallel computing on the validation of atomistic simulations software and their application in industrial ICME.

**9:50 AM**

**What Are the Challenges to Acceptance of Molecular Simulation in Engineering and Design?**: *Chandler Becker*[1]; Eric Lass[1]; [1]NIST

Molecular simulation, including molecular dynamics, is gaining in popularity and utility for understanding atomic-scale processes. However, there are numerous challenges that need to be addressed for the field to truly be an accepted part of the engineering and design process. These challenges include the rapid development, acquisition and trustworthiness of interatomic potentials; the selection of reference data to assess their accuracy; dissemination of the results; and the need to have molecular simulation compete on the timescales required by industry. In this presentation, we will discuss efforts to address these and other challenges to the industrial acceptance of molecular simulation.

**10:10 AM**

**Thermodynamic Properties of Paramagnetic Iron from Non-collinear DFT Calculations**: *Vsevolod Razumovskiy*[1]; Andrei Ruban[2]; Andrei Reyes-Huamantinco[1]; [1]Materials Center Leoben; [2]KTH Royal Institute of Technology

The recently developed Spin Wave (SW) method [1] has been applied to calculation of various thermodynamic properties of bcc and fcc paramagnetic iron. Spin-wave formalism provides a convenient alternative way of modeling the high-temperature paramagnetic state for a certain type of magnets within the framework of Hamiltonian-type electronic-structure methods. For Heisenberg systems, it is formally equivalent to the so-called disordered local moment (DLM) approach, which is usually used in the methods based on the coherent potential approximation within the Green's function or multiple-scattering techniques. Here, we present the results of SW approach based on Density Functional Theory calculations of some thermodynamic properties of paramagnetic bcc and fcc iron, including formation energies of defects and phonon spectra, obtained using Exact Muffin Tin Orbitals (EMTO) method and Projector Augmented-Wave (PAW) method as implemented in Vienna Ab-initio Simulation Package (VASP). [1] A. V. Ruban, V. I. Razumovskiy, Physical Review B 85 (2012) 174407.

**10:30 AM**

**3D Hybrid Atomistic Modeling of ß'' in Al–Mg–Si: Putting the Full Coherency of a Needle Shaped Precipitate to the Test**: *Flemming Ehlers*[1]; Stéphane Dumoulin[2]; Randi Holmestad[1]; [1]Norwegian University of Science and Technology, NTNU; [2]SINTEF, Materials and Chemistry

A key input of a truly predictive integrated computational materials engineering (ICME) scheme for an age hardenable Al alloy is the formation enthalpies – including interfacial and strain contributions – for the main hardening precipitate(s). The basic desire to compute these numbers with ab initio methods for essentially all relevant precipitate sizes continues to face limitations in the context of the associated requirements for the model system extensions. These obstacles manifest themselves in particular when considering a density functional theory framework based description of the full precipitate-host lattice interface – needed in order to incorporate accurately electronic interactions as well as the strain evolution along high misfit directions. Recent work within our group has made it possible to carry out this interface modeling for a fully coherent precipitate at a comparatively weak level of approximation. We describe here our first attempts to employ this scheme for 3D hybrid modeling of fully coherent needle-shaped ß'', the main hardening phase in the Al–Mg–Si alloy system. Examining a physically sized precipitate, we found this structure to fully adapt to the host lattice along its main growth (needle) direction, with the cell dimensions in the precipitate cross-section falling non-negligibly below the experimental values for both compositions ($Mg_5Si_6$, $Mg_5Al_2Si_4$) tested. Further, the theoretical value of 107.8° for the ß''–$Mg_5Si_6$ monoclinic angle ß_P is markedly off the experimental value of 105.3°±0.5°, potentially supporting the presence of non-negligible amounts of Al in the ß'' phase.

**10:50 AM Break**

**11:10 AM**

**First Principles Computational Determination of Anisotropic Elastic Constants of Hard Compounds (Borides) Through Density Functional Theory**: *K. S. Ravi Chandran*[1]; K. Panda[1]; [1]University of Utah

Single crystal elasticity and the anisotropy in hard compounds such as borides and others having complex crystal structures are of interest in understanding how crystallography, stoichiometry and atomic bonding determine the elasticity of crystals. In this work, we demonstrate a robust approach for the determination of anisotropic elastic constants of hard titanium borides, TiB and TiB2, using only the periodic table atomic data through the Density Functional Theory (DFT) calculations as implemented in Wien2K code. The elastic constants were determined using the Full-Potential-Linear-Augmented-Plane-Wave (FLAPW) method and the generalized gradient approximation (GGA). TiB has orthorhombic (Pnma) crystal structure, hence, there are nine independent elastic constants. TiB2 has a hexagonal structure (P6/mmm) with six independent elastic constants. A complete determination of these constants is necessary for understanding the mechanical behavior of these compounds. It is shown here that using suitable elastic lattice distortions of the unit cell the anisotropic elastic constants of these crystals can be calculated by DFT quite accurately. It is also shown that internal atomic relaxations after elastic distortions have the greatest effects on the numerical values elastic constants, thus showing the sensitivity of calculations to atomic positions. The present approach can be very useful in calculating the anisotropic elastic constants of hard to synthesize crystals and in examining how chemistry, stoichiometry and bonding affect elasticity, particularly in the search for hard ternary compounds.

**11:30 AM**

**Ab Initio Determination of Interfacial Energetics of Alloys**: *Liang Qi*[1]; Maarten de Jong[1]; Mark Asta[1]; [1]University of California, Berkeley

The plasticity and toughness of metals are strongly influenced by the energetics of specific interfacial structures, such as surface energy, unstable stacking fault energy and twin boundary energy. Alloying is an effective method to tune these interfacial energies in order to improve the mechanical performance. However, it is difficult to apply ab initio calculations to predict these energies for alloys that are not in ordered phases, because finite-size supercells cannot describe the low-symmetry crystalline systems. By applying statistical methods, we use small supercells with ~100 atoms to calculate these interfacial energies of binary alloys with different compositions. There are two general strategies to construct these small supercells: one is special quasirandom structures (SQS) to simulate the perfect random alloys; the other is cluster expansion (CE) to describe short-range ordering surrounding the interfaces. For both cases, empirical embedded-atom-method (EAM) potentials are adopted first to calculate the interfacial energies of real binary alloys in large supercells (number of atoms >> ~100), which are used as benchmarks for the small-supercell calculations. Different supercells and EAM potentials are tested in order to verify the accuracy of our methods. The small system sizes make these methods possible candidates for the ab initio determination of the interfacial energetics of substitutional alloys. This work is finally supported by the U.S. Office of Naval Research under grant number N00014-11-1-0886.

**11:50 AM**

**Molecular Dynamics and Experimental Characterization of Martensitic Transformations in CoNiAl Alloys**: Vesselin Yamakov[1]; *Terryl Wallace*[2]; John Newman[2]; Ganga Purja Pun[3]; Yuri Mishin[3]; [1]National Institute of Aerospace; [2]NASA Langley Research Center; [3]George Mason University

Molecular dynamics simulations with a recently developed embedded-atom interatomic potential are used to study the effect of chemical composition and uniaxial mechanical stresses on the martensitic phase transformation in CoNiAl alloys. The transformation is analogous to the martensitic transformation in Ni-rich NiAl alloys. The martensitic phase has a tetragonal crystal structure and can contain multiple twins arranged in domains of different orientations in a crystal. The predicted martensitic transformations are compared to experimental data obtained from CoNiAl arc-melted buttons fabricated with various compositions. Specimens were machined from these buttons, solution-treated and quenched to lock in the shape-memory behavior, and then the martensitic transformation was characterized using differential scanning calorimetry (DSC) and electron microscopy. The simulation model shows similarities, but also some differences with the experimental data. The temperature and the hysteresis of the transition in the simulation model tend to be higher than the experimental values and are shown to depend strongly on the configurational entropy of the system, which is estimated by using grand-canonical Monte Carlo simulations. The simulation model also indicates a decrease in the transition temperature with increase in the Co concentration, which is in agreement with the experimental data.

**12:10 PM**

**Site Preference and Interaction Energies of Co and Cr in Gamma Prime $Ni_3Al$: A First Principles Study**: *Jincheng Du*[1]; Mrunal Chaudhari[1]; [1]University of North Texas

Nickel based superalloys have been critical for aerospace and power applications due to excellent high temperature properties. These high temperature properties have been attributed to the coherently precipitated gamma prime phase in the gamma matrix. The segregation of alloying elements between the matrix and gamma prime phase drives precipitate misfit strains and impacts material strength. This study aims at understanding the site preference of Co and Cr within the ordered gamma prime phase. The study also calculates the interaction energy between alloying additions within the ternary systems Ni-Al-Cr and Ni-Al-Co, and the quaternary system Ni-Al-Cr-Co. Results show that the Co shows a mixed substitution behavior between the Al and Ni sites in the gamma prime phase. The results from Ni-Al-Cr ternary system shows that two Cr atoms favor being close to each other, with the most stable configuration of first nearest neighbors of Al-Al site. The interaction energies calculated from the Ni-Al-Co system show that the initial distance between two Co atoms will decide if the two Co atoms prefer Ni-Ni or Ni-Al configuration. The study on the quaternary system Ni-Al-Cr-Co reveals that the initial configuration of Cr and Co atoms will affect the final most stable configuration. The results were found to be consistent with our previous findings.

**12:30 PM**

**Online Atomistic Polymer Simulations at NanoHUB.org**: *Benjamin Haley*[1]; Chunyu Li[1]; Nathaniel Wilson[1]; Eugenio Jaramillo[2]; Alejandro Strachan[1]; [1]Purdue University; [2]Texas A&M International University

The lack of easy access to powerful simulations and lack of a workforce trained on computer simulations of materials are important factors limiting the adoption of ICME in industry. NSF's nanoHUB.org is a web-portal that enables users to perform online simulations using simply a web-browser. With over 200 simulation tools freely available and high-quality online training and educational material, nanoHUB.org can play an important role making simulation tools widely accessible and training a new generation of engineers familiar with ICME tools. In this presentation we describe PolymerModeler, a nanoHUB.org tool that offers a free platform for research and education in atomistic polymer simulations. The tool allows users to construct and visualize atomistic models of thermoplastic polymers. The mechanical properties of the resulting systems may be studied using LAMMPS, within the PolymerModeler tool. LAMMPS simulations run on NSF-funded HPC resources, and the results display in the web browser. Users do not need to download or install any software. A first time user guide introduces the tool and common usage scenarios. The polymer builder section of the tool constructs chains by adding successive monomers. Several pre-built monomers are available, and users can upload any repeated unit, in PDB or XYZ format, making it a very general amorphous builder.

## ICME Building Blocks: Computational Thermodynamics and Kinetics

Wednesday PM Room: Ballroom D
July 10, 2013 Location: Salt Lake Marriott Downtown at City Creek

*Session Chairs:* Paul Jablonski, US Department of Energy; Paul Mason, Thermo-Calc Software Inc.

**2:30 PM**

**The Role of the CALPHAD Approach in ICME**: *Fan Zhang*[1]; Weisheng Cao[1]; Shuanglin Chen[1]; Chuan Zhang[1]; Jun Zhu[1]; [1]CompuTherm, LLC

Adjusting materials chemistry and processing conditions have been a common practice of materials scientists/engineers in the design of new materials and the improvement of the existing materials. Traditional approaches relying on trial-and-error are no longer viable due to limited resources. Integrated Computational Materials Engineering (ICME), which integrates materials information obtained from computational tools with engineering product performance analysis, has recently been highlighted as a methodology that can unlock great potential for significant benefits in cost-effective materials and process design. CALPHAD, which emerged first as an approach for the calculation of phase equilibria and thermodynamic properties of complex multi-component, multi-phase systems, has in recent years been applied to a broader field of materials science and engineering beyond phase diagrams, such as solidification, coating, joining, and phase transformation. The software developed based on this approach has become a generic tool available to ICME practitioners. In this presentation, I will discuss the role of CALPHAD approach in ICME. I will use examples to demonstrate how it can be integrated with key experiments in accelerating materials design and development under the framework of ICME. I will also demonstrate how this approach can further extend its application by integrating with kinetic models and property models. In particular, I will focus on the integration of thermodynamic calculation with precipitation simulation for the understanding of precipitation behavior and age hardening effect during heat treatment processes. Nickel-based superalloys and aluminum alloys will be used as examples throughout the presentation.

**2:50 PM**

**An Open Source Thermodynamic Software and Database Structure as Backbone for Application Software in Materials Science**: *Bo Sundman*[1]; Ursula Kattner[2]; Mauro Palumbo[3]; Suzana Fries[3]; [1]CEA Saclay; [2]NIST; [3]ICAMS, RUB

Calphad thermodynamic software and databases are important tools for materials and processing development as they can calculate properties outside the equilibrium state. An obstacle to wide application and further development of the Calphad technique is that most software and databases are proprietary and cannot be modified or easily integrated into new applications by users. In this presentation the "Open Calphad"(OC) initative will be described which offers high quality free software and a flexible database structure. The software has an easily extendable facility for users to include modeling of any kind of phase property as function of temperature, pressure and phase constitution of a material. A large

number of models for the composition dependence of different kinds of phases have been developed within the Calphad community which will be available within OC. The OC initiative has also the ambition to provide high quality assessments of key binary and ternary systems.

**3:10 PM**

**Assessment of Thermodynamic Data by Physically-based Thermo-kinetic Modeling**: *Erwin Povoden-Karadeniz*[1]; Peter Lang[2]; Ernst Kozeschnik[3]; [1]Vienna University of Technology, CDLESOP; [2]Materials Center Leoben Forschung GmbH; [3]Vienna University of Technology, Institute of Materials Science and Technology

Computational thermo-kinetic simulation has become a standard technique in order to understand nucleation, growth and dissolution of precipitates in a super-saturated solid solution. If one utilizes a precipitation simulation approach that is based on parameter-free physical models such as, for instance, the generalized broken-bond model for evaluation of the interfacial energy in solid-state nucleation theory, and the SFFK model describing the evolution of particle size and composition during arbitrary thermo-mechanical treatments, these models allow for a refinement of parameters in the assessment of equilibrium thermodynamic free energy parameters. In the case of metastable phases, fast and efficient approximation of properties such as the entropy of formation is attainable that would otherwise require time-consuming and difficult computational techniques based on first-principles calculation. In this work, it is demonstrated that our approach leads to reasonable trends in formation entropies for a sequence of metastable precipitates. Case studies in Al-Mg-Si alloys and in Ti-Ni shape memory alloys are presented.

**3:30 PM**

**Thermodynamic and Kinetic Simulation and Experimental Results Homogenizing Advanced Alloys**: *Paul Jablonski*[1]; Jeffrey Hawk[1]; [1]US Department of Energy

In nearly all metal alloys, segregation occurs during solidification because some solute elements partition preferentially to the liquid while others partition to the solid. Many cast articles are subjected to a homogenization heat treatment in order to minimize or eliminate the as-cast segregation and thus improve their hot working characteristics if wrought processed or in-service performance if used as a casting. Traditionally, the homogenization heat treatment is based either upon past practice on related alloys or uses many time consuming laboratory experiments based on a trial and error approach. Through the use of thermodynamic and kinetic modeling software, NETL has designed a systematic method that has been successfully developed to design an optimized homogenization heat treatment that eliminates chemical segregation that occurs across secondary dendrite arms within a cast microstructure. It allows the researcher to homogenize a casting to a level suitable for the application at hand as well as to adjust temperatures and times to fit their in-house equipment (capability, reliability, etc.) or work schedule. In this approach, the Scheil module within Thermo-Calc is used to predict the as-cast segregation present within an alloy, and then DICTRA (Diffusion Controlled TRAnsformations) is used to model homogenization kinetics as a function of time and temperature. Thus, in this presentation the computationally designed heat treatment, and the subsequent verification of its success in eliminating the chemical segregation present within the microstructure of real castings, is presented.

**3:50 PM**

**Optimizing Alloy and Process Design Using Thermodynamic and Properties Databases and a Direct Search Algorithm**: *Aimen Gheribi*[1]; Eve Belisle[1]; Christopher Bale[1]; Sebastien Le Digabel[1]; Charles Audet[1]; Arthur Pelton[1]; [1]Ecole Polytechnique de Montreal

The FactSage thermodynamic databases contain data for thousands of compounds and multicomponent solution phases for steel, light metals, oxides, salts, etc. They have been prepared by critical evaluation and modeling of available thermodynamic and phase equilibrium data. They also contain critically evaluated and modeled densities, expansivities and liquid viscosities for many systems. The FactSage software can access these databases to calculate phase diagrams and the conditions for phase equilibria, follow the course of equilibrium or Scheil-Gulliver cooling, etc. In alloy and process design, one often seeks to identify compositions where certain functions have optimal values under various constraints. Such functions include liquidus temperature, amounts and compositions of phases, densities, vapor pressures, viscosities, etc. We report here on a software package called FactOptimal, linked through a user interface to the FactSage software and databases, to perform such calculations. The software incorporates the Mesh Adaptive Direct Search algorithm which is designed for non-smooth multi-objective optimization problems. As well as optimizing functions calculated directly by FactSage, FactOpimal can optimize other properties such as tensile strength, yield strength, grain size, thermal conductivity, etc. which can be related to the calculated equilibrium properties (such as the amounts and compositions of the phases) for specific conditions (such as cooling rate, annealing time and temperature, etc.) through user-supplied functions. Several examples of applications to alloy and process design will be presented. The possibility of eventually linking FactOptimal to other existing properties databases will be discussed.

**4:10 PM Break**

**4:30 PM**

**Simulations of Precipitate Microstructure Evolution during Heat Treatments**: *Kaisheng Wu*[1]; Gustaf Sterner[2]; Qing Chen[2]; Herng-Jeng Jou[3]; Johan Jeppsson[2]; Johan Bratberg[2]; Anders Engstrom[2]; Paul Mason[1]; [1]Thermo-Calc Software Inc; [2]Thermo-Calc Software AB; [3]QuesTek Innovations LLC

Precipitation, a major solid state phase transformation during heat treatment processes, has for more than one century been intensively employed to improve the strength and toughness of various high performance alloys. Recently, sophisticated precipitation reaction models, in assistance with well-developed CALPHAD databases, provide an efficient and cost-effective way to tailor precipitate microstructures that maximize the strengthening effect via the optimization of alloy chemistries and heat treatment schedules. In this presentation, we focus on simulating precipitate microstructure evolution in Nickel-base superalloys under arbitrary heat treatment conditions. The newly-developed TC-PRISMA program has been used for these simulations, with models refined especially for non-isothermal conditions. The effect of different cooling profiles on the formation of multimodal microstructures has been thoroughly examined in order to understand the underlying thermodynamics and kinetics. Meanwhile, validations against several experimental results have been carried out. Practical issues that are critical to the accuracy and applicability of the current simulations, such as modifications that overcome mean-field approximations, compatibility between CALPHAD databases, selection of key parameters (particularly interfacial energy and nucleation site densities), etc., are also addressed.

**4:50 PM**

**Development of Gradient Cemented Carbides through ICME Strategy**: *Yong Du*[1]; Yingbiao Peng[1]; Weibin Zhang[1]; Weimin Chen[1]; Peng Zhou[1]; Wen Xie[2]; Kaiming Cheng[1]; Lijun Zhang[1]; Guanghua Wen[2]; Shequan Wang[2]; [1]State Key Lab of Powder Metallurgy, Central South University; [2]Zhuzhou Cemented Carbide Cutting Tools Limited Company

Thermodynamic and diffusivity databases for multi-component C-Co-Cr-W-Ta-Ti-Nb-N cemented carbides have been developed through a combination of assessment and experimental work. The thermodynamic database is based on previous thermodynamic descriptions of all of the binary systems and most of the ternary systems. Some of the ternary systems are assessed according to experimental data or reassessed due to the refinement of binary systems. The diffusivity database contains the atomic mobility parameters for technologically important phases, such as liquid, WC, carbides and nitrides. The Sutherland equation is modified in the present work to predict both self- and impurity diffusivities in liquid. The atomic mobility of fcc phase is assessed by means of electron probe microanalysis (EPMA) and semi-empirical equation. Gradient cemented carbides WC-Ti(C,N)-TaC-Co, WC-Ti(C,N)-NbC-Co, WC-Ti(C,N)-TaC-NbC-Co sintered under vacuum and WC-Ti(C,N)-Co sintered under various partial pressures of N2 have been prepared. The microstructure of the gradient zone is investigated via scanning electron microscopy (SEM). The concentration profile is determined by means of EPMA. The influence of carbon content and N2 partial pressure on the formation of the gradient zone has been investigated. Base on the established databases, the microstructure evolution during sintering of cemented carbides is simulated using the phase field method. The simulation results agree well the present experimental data and literature data. The genome schematic diagram for the development of gradient cemented carbides is proposed.

**5:10 PM**

**Computational Study of Pearlite Growth in Mixed Diffusion-controlled Regime**: *Kumar Ankit*[1]; Britta Nestler[1]; [1]Institute of Materials and Processes, Karlsruhe Institue of Technology

We investigate the complex lamellar growth of pearlite in austenite, during the eutectoid transformation in steel, using a modified multi-phase-field model [1] (the grand-potential formulation). First, we extend the Jackson-Hunt-type calculation, done previously for eutectic transformation, to eutectoid transformation by accounting for diffusion in austenite as well as ferrite. It is predicted, that carbon diffusion from austenite and ferrite leads to the formation of tapered cementite along with an overall increase in the transformation kinetics as compared to growth from austenite (only). The difference in the dynamics is described by a factor 'ρ' which comprises of the ratio of the diffusivities of the bulk and the growing phases, along with the ratios of the slopes of the phase co-existence lines. Next, we approximate the variation of grand-potential for respective phases as a function of chemical potential by utilizing information from the CALPHAD database (for Fe-C system) and carry out the phase-field simulations to test the accuracy of analytically derived velocity (as a function of lamellar spacing and undercooling). Further, we also study the influence of grain boundary diffusion on the pearlite growth rate and make an integrated comparison of phase-field simulation results with experiments. Reference: [1] A. Choudhury and B. Nestler. Grand-potential formulation for multicomponent phase transformations combined with thin-interface asymptotics of the double-obstacle potential. Phys. Rev. E, 85:021602, 2012.

**5:30 PM**

**Phase-field Modeling of Microstructure Evolution in Nuclear Fuels under Elastic-plastic Deformation**: *Shenyang Hu*[1]; Yulan Li[1]; Xin Sun[1]; [1]Pacific Northwest National Laboratory

Predicting microstructure and property evolution in materials is one of key elements in Integrated Computational Materials Engineering (ICME). In this talk, we will present a phase-field model for investigating microstructure evolution in an elastic-plastically inhomogeneous solid. In particular, we study the evolution kinetics of gas bubbles or voids in nuclear fuels under elastic and plastic deformation. The model takes into account vacancy and gas atom diffusion as well as the coupling of diffusion and deformation. All lattice mismatches associated with point defects and plastic deformation are described using the micromechanics concept of space-dependent "stress-free" or "eigen" strains. Iteration methods are used to find the elastic and plastic solution. The effect of the thermal stresses due to the temperature gradient in the nuclear fuels on nucleation, growth and coarsening behaviors of gas bubbles or voids will be presented and discussed in the talk.

## ICME Building Blocks: Process and Performance Modeling

Wednesday PM Room: Ballroom E
July 10, 2013 Location: Salt Lake Marriott Downtown at City Creek

*Session Chairs:* Veera Sundararaghavan, University of Michigan; Matthias Militzer, University of British Columbia

**2:30 PM**

**Microstructure-based Modeling and Experimental Validations of Dislocation and Twinning Plasticity in Metals**: *Jaafar El-Awady*[1]; [1]Johns Hopkins University

Extrinsic size-effects in metals and alloys have been a rich topic of research over the past decade, and continue to grow with numerous new challenges and questions emerging at the micro- and nano-scales. We combine large scale atomistic simulations, discrete dislocation dynamics (DDD) simulations and microscale experiments to identify the mechanisms governing size-scale effects. Previous experimental studies, limited to a very small subset of starting initial dislocation densities and microcrystal sizes (mostly submicron), suggest that Taylor hardening law fails at micron and submicron length scale. However, DDD simulations of crystals sizes over two orders of magnitude and with initial dislocation density spanning over four orders of magnitude show for the first time that a strength-dislocation density relationship exists at the macoscale as well as the microscale. Taylor hardening is also recovered above a size-dependent critical dislocation density. Microscale experiments validating these simulations are also presented. We discuss the role of this predicted critical dislocation density in controlling the size-affected flow response, and rationalize the results based on the stochastic of the dislocation network both in single and polycrystals. Results of these simulations are incorporated into a size-dependent constitutive model for crystal plasticity. Finally, atomic processes controlling size-scale effects on dislocation/twinning deformation in hexagonal packed single crystals are evaluated. These simulation tools provide a unique predicting capability to serve as a fundamental building block of ICME.

**2:50 PM**

**A Study for the Constitutive Model of Stainless Steel Subjected to High Strain Rate and Temperature**: *Yu Jianchao*[1]; Jiang Feng[1]; Rong Yiming[1]; [1]Tsinghua University

In this paper, a modified Split Hopkinson Pressure Bar with synchronically assembled heating system was employed to study the thermo-mechanical deformation behavior of Fe-Cr-Ni stainless steel subjected to dynamic compressive loading. The investigated strain rates range from 1100 to 8000s-1 while the temperatures range from room temperature (20°C) to 800°C. Quasi-static compressive experiment at room temperature was performed by servohydraulic testing machine as a comparison. The experimental results showed the flow stress was strain rate and temperature sensitive evidently, i.e., the flow stress decreases with the decrease of strain rate and increase of deformation temperature. In addition, a phenomenological constitutive model was proposed for the purpose of numerical simulation in the engineering application. The specific heat capacity in different temperatures was measured to accurately

model the flow stress thermal softening caused by adiabatic temperature rise. The proposed constitutive model is validated by compared with the experimental results. The analytical predictions showed good agreement with experimental results, which confirmed the proposed constitutive model can give an accurate estimate of the flow stress in the strain rate and temperature ranges investigated.

**3:10 PM**

**Full-field Multi-scale Modelling of Sheet Metal Forming Taking the Evolution of Texture and Plastic Anisotropy into Account**: *Paul Van Houtte*[1]; Jerzy Gawad[2]; Eyckens Philip[1]; Albert Van Bael[1]; Giovanni Samaey[1]; Dirk Roose[1]; [1]KULeuven; [2]AGH University of Science and Technology

Focus is on the implementation of texture-induced plastic anisotropy in FE simulations of metal forming. The crystallographic texture can be introduced as a state variable in every integration point. A multi-scale model is then called to calculate the stress-strain response and the local texture evolution in every integration point and for every strain increment. Less calculation-intensive is to use anisotropic analytical constitutive models, identified in advance from mechanical tests. These can also be done in a "virtual" way, i. e. using measured texture data and a multi-scale model. However, texture evolution is then not taken into account. An adaptive scheme for updating the texture and the anisotropy has been developed recently. Texture and anisotropy were updated by the ALAMEL-model. Results for a some sheet metal forming processes are shown. The calculation times had been reduced from months to days. Predicted fields of plastic anisotropy and textures are discussed including experimental validation.

**3:30 PM**

**Integrating Quench Modeling into the ICME Workflow**: Andrew Banka[1]; *Jeffrey Franklin*[1]; William Newsome[1]; [1]Airflow Sciences Corporation

ICME offers the promise of accelerating design cycles while improving the performance of manufactured components. In order for ICME to be effective, all portions of the design, materials specification, and manufacturing process need to be included in the analysis. Heat treating, including a liquid or gas quenching step, is an integral component of the production of most metal components. The rapid cooling that occurs during quenching largely defines the phase distribution, microstructure, residual stress, and distortion in the as-quenched part. While Computational Fluid Dynamics (CFD) can predict the heat fluxes during gas quenching operations, the complexity of phase change boiling phenomena makes the prediction of liquid quenching operations difficult. For this reason, the quenching process is often omitted from the ICME workflow. Development of suitable CFD boiling models for practical heat treating operations requires the collection of relevant data and development of correlations that reflect that observed behavior. While significant work has been done in this area for nucleate boiling of water at saturated conditions, additional data is needed to cover the full range of boiling regimes, other quench liquids (e.g., oil and polymer), and subcooled conditions. In order to collect the data needed to develop improved CFD boiling models, an experimental facility has been constructed. A description of the test facility is providing along with data collected for a range of boiling conditions. Speculation on the form of correlations and implementation into CFD codes are also included.

**3:50 PM**

**Modeling Crack Propagation in Polycrystalline Alloys using Crystal Plasticity Finite Element Method**: *Veera Sundararaghavan*[1]; Shang Sun[1]; [1]University of Michigan

Crack propagation in polycrystalline grains is analyzed using a novel multiscale polycrystalline model. The approach combines reduced order descriptors of microstructures with explicit representation of polycrystals at critical areas (eg. crack tips). For the critical areas, refined meshes are employed to discretize each crystal. The crack propagation in the microstructure is calculated using the variational multiscale method which allows for arbitrary transgranular and intergranular crack paths. As the crack propagates, the global ODF (at the macroscale) evolves to new state following a Lagrangian algorithm proposed in our previous work. The computational load is reduced substantially by combining probabilistic representation of the macroscale problem with exact resolution of the crystals at the crack tips. Several example problems are demonstrated showing exceptional mesh convergence and efficiency of the numerical approach.

**4:10 PM Break**

**4:30 PM**

**A Coupled Approach to Weld Pool, Phase and Residual Stress Modelling of Laser Direct Metal Deposition (LDMD) Processes**: *Mustafa Megahed*[1]; Mushtaq Khan[2]; Juansethi Ibara-Medina[2]; Michael Vogel[2]; Narcisse N'Dri[1]; Andrew Pinkerton[3]; [1]ESI Group; [2]University of Manchester; [3]Lancaster University

This paper describes a CFD model of the laser metal deposition process coupled with a metallurgical grain structure tool and a stress solver to determine residual stresses. The model covers the complete process, starting from the simulation of powder particles in the deposition head and finishing with the final part. Individual phenomena that are considered in the gas-phase stage of the model include the ricocheting of particles within the head, the flow of powder particles, their interaction with the laser and powder catchment/bouncing. Phenomena considered in the liquid phase (melt pool) stage of the model include particle enthalpy effects, buoyancy, temperature-dependent material properties and Marangoni forces. The CFD model is coupled with a metallurgical data base to predict the phase and material properties of the solidified deposit and heat affected area and residual stresses in the part. Modelled and experimental characteristics of multi-track deposits of M2 steel show good agreement.

**4:50 PM**

**Process Model for Accelerated Cooling of Hot-rolled Low-carbon Steels**: *Matthias Militzer*[1]; Vladan Prodanovic[1]; Tao Jia[2]; Thomas Garcin[1]; [1]The University of British Columbia; [2]Northeastern University

Accelerated cooling on the run-out table of a hot mill is a key technology to produce advanced hot-rolled steel sheets and plates with improved properties for applications in the automotive, construction and energy industries. A run-out table process model has been developed that integrates cooling and phase transformation models. The phenomenological temperature model has been formulated based on dedicated heat transfer studies on a pilot scale run-out table. The transformation model predicts the austenite decomposition into complex multi-phase microstructures including ferrite, pearlite, bainite and martensite for selected advanced low-carbon steels. The theoretical treatment of the austenite decomposition has been aided by a multi-scale modeling approach utilizing atomistic and phase field simulations. In particular, this approach enabled to describe solute drag of substitutional alloying elements, e.g. Mn and Nb, on migrating austenite-ferrite interfaces with a physically based model. Structure-property relationships are employed to link the predicted microstructure to the resulting mechanical properties. Status and challenges of run-out table process model development and validation will be reviewed.

**5:10 PM**
**Prediction of the Uncertainty in the Response of Lightweight Structures Consisting of Solid Foams**: *Jörg Hohe*[1]; Carla Beckmann[1]; [1]Fraunhofer-Institut für Werkstoffmechanik IWM

Solid foams are important core materials in sandwich construction combining a rather low spe-cific weight with a reasonable stiffness and strength. Further benefits derive from their inherent good thermal and acoustic damping characteristics. On the other hand, their main disadvantage is their disordered random microstructure leading to a distinct scatter in their effective properties and thus uncertainties in the response of the entire structure. The present study is concerned with a numerical scheme for prediction of the uncertainties in the mechanical response of sandwich or other lightweight structures made at least partially of solid foams using an integrated two-step procedure. In a first step, the effective material properties of the solid foams and their uncertainty are determined. For this purpose, a proba-bilistic homogenization procedure is established, based on the analysis of the mechanical re-sponse of small scale "testing volume elements", defined as subsets of a large scale, statisti-cally representative volume element. As a result, the probability distributions for the effective properties and the autocorrelation properties for a random field description of the effective material response of the solid foam are obtained. In a second step, the random field model is employed in a numerical analysis of the entire structure on the macroscopic level. In a case study, a single edge clamped sandwich beam with a foam core is considered. Whereas the material uncertainty is found to cause only minor scatter in the deformation of the beam, significant uncertainties are observed in the strength of the considered structure.

## ICME Challenges and Education

Thursday AM Room: Ballroom D&E
July 11, 2013 Location: Salt Lake Marriott Downtown at City Creek

*Session Chairs:* James Warren, National Institute of Standards and Technology; Baicheng Liu, Tsinghua University

**8:00 AM Introductory Comments:** Katsuyo Thornton, University of Michigan

**8:05 AM Invited**
**Enabling Elements of Integrated Computational Materials and Manufacturing Science and Engineering (ICM2SE)**: *David Furrer*[1]; [1]Pratt & Whitney

Application of computational materials and manufacturing science and engineering has continued to grow and evolve toward an integrated engineering discipline. The speed of this integration is increasing through the efforts within many supporting technologies that have previously kept the pull for the anticipated significant ICM2SE benefits in check. Enabling technologies in the areas of advanced physics-based models, computational methods, materials and process data availability and management, and standards are leading to clear paths toward true integration of computational material and manufacturing science and engineering with other engineering disciplines. The complexity and overall interdisciplinary nature of ICM2SE must be thought about with a "systems engineering" approach with clear objectives and subsequent assemblages of appropriate tools and methods. The enabling elements of ICM2SE technology that are resulting in the rapid changes to the ICM2SE landscape will be presented and discussed from the perspective of industrial application. Examples of integrated computational materials and manufacturing engineering will be provided to show the increasing complexity and rate of use of this technology to support advanced component and product design, optimization and realization.

**8:35 AM**
**ICME – A Mere Coupling of Models or a Discipline on Its Own?**: Markus Bambach[1]; *Georg Schmitz*[1]; Ulrich Prahl[1]; [1]RWTH Aachen University

What is ICME? Technically, ICME is considered as an approach for solving particular engineering problems related to the design of new materials and processes by combining individual materials and process models. This combination of models is presently mostly achieved by transforming the output of a simulation to form the input for a subsequent one, which may be performed either at a different length scale or which constitutes a subsequent step along the process chain. Is ICME thus just a synonym for the coupling of simulations? In fact, most publications related to ICME are examples of the combined application of selected models and software codes to solve a specific problem. Coupling of individual models and/or software codes across length scales and along materials processing chains, however, leads to the formation of much more complex meta-models being independent of a specific application scenario. Such meta-models comprise scientific/technological aspects like e.g. standardization issues, a global reference frame, propagation of uncertainty, data contingency etc. as well as organizational aspects like e.g. distributed simulations, licensing issues in case of commercial models, suitable hardware environments and others. The viability of such meta-models thus has to be ensured by joint efforts from science, industry, software developers and independent organizations. This paper outlines several developments that seem mandatory to make ICME simulations viable, sustainable and widely accessible. As a conclusion, ICME is identified as being more than a multi-disciplinary subject but as a discipline on its own, for which a generic structural framework has to be established.

**8:55 AM**
**Knowledge Assisted Integrated Design of a Component and its Manufacturing Process**: *BP Gautham*[1]; Nagesh Kulkarni[1]; Danish Khan[1]; Pramod Zagade[1]; Rohith Uppaluri[1]; Sreedhar Reddy[1]; [1]TRDDC, Tata Consultancy Services

Linking the simulation tools used for product design, performance evaluation and its manufacturing processes in a closed loop on a single platform, along with appropriate databases and knowledge bases (e.g. rule base) would help reduce the total cost of product as well as its cost of development. Making such a knowledge assisted simulation-based design platform accessible to product or process designers, who may not possess skills for the use of simulation tools or some aspects of the design life-cycle, would help reduce the life cycle of product development further. In this paper, we propose a process and illustration for achieving an integrated product and manufacturing process design assisted by knowledge support for the user to make decisions at various stages. A case of design of transmission components is illustrated in detail. The example illustrates the design of a gear for its geometry, material selection and its manufacturing processes, particularly, carburizing-quenching and tempering and feeding the material properties predicted during heat treatment into performance estimation in a closed loop. It also identifies and illustrates various decision stages in the integrated life cycle and discusses the use of knowledge engineering tools such as rule-based guidance, to assist the designer make informed decisions. Simulation tools developed on various commercial, open-source platforms as well as in-house tools along with knowledge engineering tools are linked to build a framework with appropriate navigation through user-friendly interfaces. This is illustrated through examples in this paper.

**9:15 AM Break**

**9:35 AM Invited**

**Integrated Computational Materials Education**: *Mark Asta*[1]; Katsuyo Thornton[2]; [1]University of California, Berkeley; [2]University of Michigan

The growing importance of integrated computational materials engineering (ICME) has led to rapid progress in the development of computational methods and associated software tools for predictive modeling of processing-structure-properties-performance links in materials design and production. To date, however, the introduction of these tools into materials science and engineering curriculum has generally not kept pace. This talk will provide an overview of approaches to bridging this gap, in the training of the future ICME workforce. Two categories of approaches related to ICME education will be discussed: the development of professional degree programs, and the incorporation of computational methods into traditional MSE courses. To enable efforts in the second category, the authors have been involved in the development of a summer-school program aimed at "educating the educator." Based on input from employers, department chairs and faculty members, this summer school has focused on the development of a standard set of lecture notes and computational modules that lower the barrier for introduction of computational tools in traditional undergraduate courses. The assessed impact of these efforts will be reviewed, based on surveys from alumni of the summer school over the past two years.

**10:05 AM**

**Integrated Computational Materials Engineering (ICME): Education and Workforce Development**: Mark Horstemeyer[1]; *Nitin Sukhija*; Tomasz Haupt[1]; [1]Mississippi State University

Although Integrated Computational Materials Engineering (ICME) has recently been advocated by the National Academies as a potential to transform manufacturing related to materials processing in our country, it has yet to be fully diffused into industry. ICME entails cradle-to-grave history modeling and multiscale modeling of a material through its manufacturing process and in-service life; however, the tech transfer from the few researchers who have conducted ICME studies has not occurred. This presentation introduces a methodology to help diffuse the ICME technologies to academia and to industry. Anybody who wants to instruct/teach others about ICME tools; who wants to introduce a course at their school; or who wants to teach industry researchers and designers would have an interest in this presentation. Examples of ICME case studies will be presented as well as information to a self-contained course that can be used on-line. The on-line course has associated powerpoint lectures and access to ICME tools(www//icme.hpc.msstate.edu). This website was developed to help new students and researchers apply the ICME tools and integrate their experimental data with the modeling methodologies. It is a wiki-based website, so researchers can add their information and realize greater impact related to their research as well as learn more rapidly from the tutorials, etc. An associated course was first taught in Fall 2012 at Mississippi State University. The book entitled "Integrated Computational Materials Engineering (ICME) for Metals: Introducing Multiscale Modeling to Invigorate Engineering Design with Science" was designed for students to learn the history, methods, and systemization procedures.

**10:25 AM Break**

**10:35 AM Panel Discussion**

**11:25 AM Concluding Comments**

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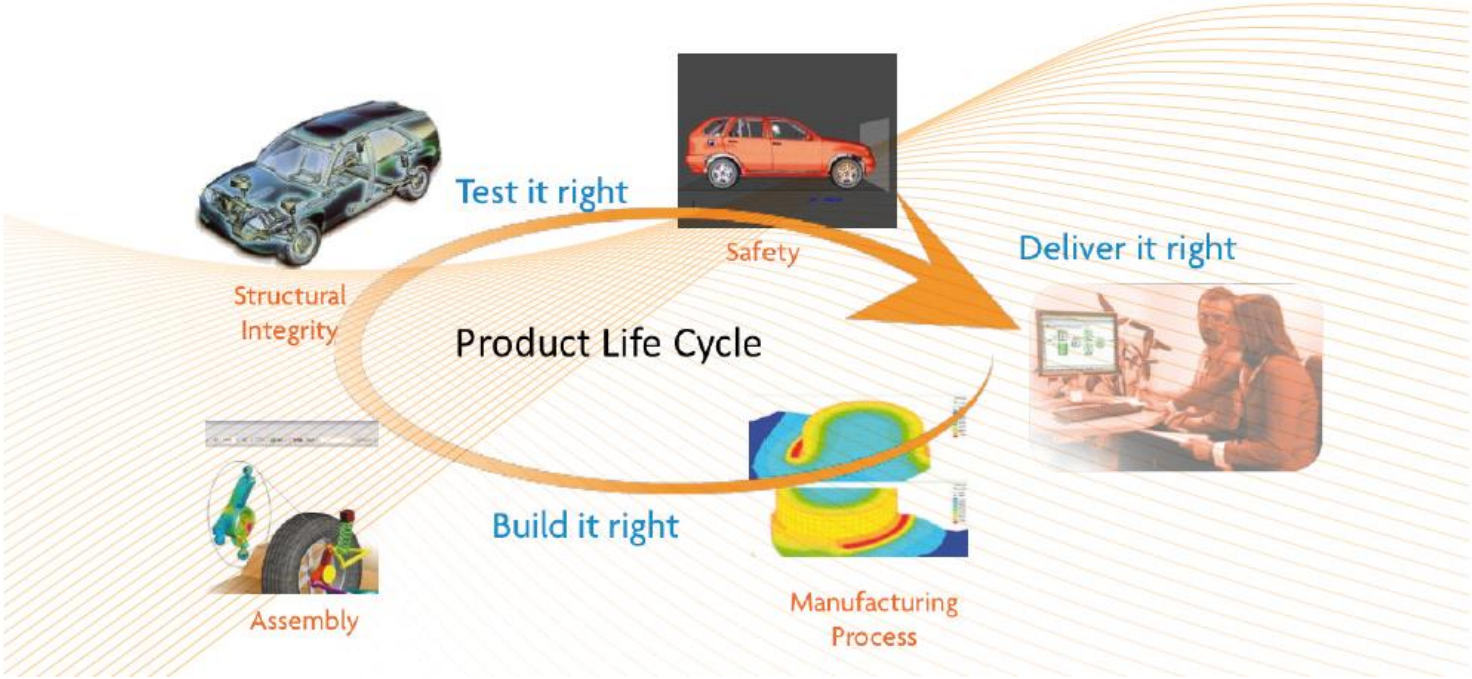


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