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3rd World Congress on Integrated Computational Materials Engineering (ICME 2015)

Cheyenne Mountain Resort • Colorado Springs, Colorado, USA

FINAL PROGRAM

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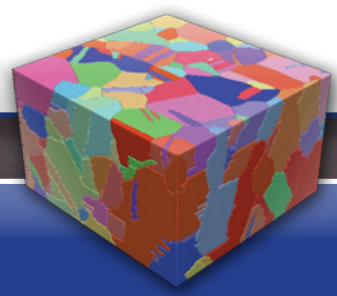

www.tms.org/ICME2015

EVENTS SCHEDULE & TABLE OF CONTENTS

SCHEDULE OF EVENTS

Sunday, May 31

Registration	5:30 p.m. to 7:30 p.m.	Lower Lobby
Welcome Reception	6:30 p.m. to 7:30 p.m.	Colorado Gallery

Monday, June 1

Registration	7:30 a.m. to 6:00 p.m.	Lower Lobby
Technical Sessions	8:00 a.m. to 10:00 a.m.	Colorado II & III
Break	10:00 a.m. to 10:20 a.m.	Colorado Gallery
Exhibition Set-up	9:00 a.m. to 12:00 p.m.	Colorado I
Technical Sessions	10:20 a.m. to 12:20 p.m.	See pages 11-14 for locations
Lunch Break	12:20 p.m. to 2:00 p.m.	On Your Own
Technical Sessions	2:00 p.m. to 5:00 p.m.	See pages 15-22 for locations
Exhibition	3:00 p.m. to 4:00 p.m. 5:00 p.m. to 6:30 p.m.	Colorado I
Break	3:20 p.m. to 3:40 p.m.	Colorado Gallery
Poster Session I and Reception	5:00 p.m. to 6:30 p.m.	Colorado I

Tuesday, June 2

Registration	7:30 a.m. to 6:00 p.m.	Lower Lobby
Technical Sessions	8:00 a.m. to 12:00 p.m.	See pages 23-28 for locations
Break	9:40 a.m. to 10:00 a.m.	Colorado I
Exhibition	9:00 a.m. to 11:00 a.m. 3:00 p.m. to 6:30 p.m.	Colorado I
Lunch Break	12:00 p.m. to 2:00 p.m.	On Your Own
Technical Sessions	2:00 p.m. to 3:30 p.m.	Colorado II & III
Break	3:30 p.m. to 4:00 p.m.	Colorado I
ICME Tools Showcase	4:00 p.m. to 5:00 p.m.	Colorado II & III
Poster Session II and Reception	5:00 p.m. to 6:30 p.m.	Colorado I

Wednesday, June 3

Registration	7:30 a.m. to 5:00 p.m.	Lower Lobby
Technical Sessions	8:00 a.m. to 10:00 a.m.	Colorado II & III
Break	10:00 a.m. to 10:20 a.m.	Colorado I
Exhibition	10:00 a.m. to 12:00 p.m.	Colorado I
Technical Sessions	10:20 a.m. to 12:40 p.m.	See pages 34-37 for locations
Break	11:20 a.m. to 11:40 a.m.	Colorado I
Lunch Break	12:40 p.m. to 2:00 p.m.	On Your Own
Technical Sessions	2:00 p.m. to 5:00 p.m.	See pages 38-42 for locations
Exhibition Dismantle	12:00 p.m. to 3:00 p.m.	Colorado I
Congress Dinner	6:00 p.m. to 8:00 p.m.	Remington I & II

Thursday, June 4

Registration	7:30 a.m. to 12:00 p.m.	Lower Lobby
Technical Sessions	8:00 a.m. to 12:00 p.m.	Colorado II & III
Break	9:10 a.m. to 9:20 a.m. 10:10 a.m. to 10:30 a.m.	Colorado Gallery
Short Course Registration	12:00 p.m. to 1:00 p.m.	Lower Lobby
Short Course: Implementing ICME in Industry	1:00 p.m. to 4:30 p.m.	Amphitheater (EPR) area

Friday, June 5

Continuation of Short Course: Implementing ICME in Industry	8:30 a.m. to 4:30 p.m.	Amphitheater (EPR) area

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3rd World Congress on Integrated Computational Materials Engineering (ICME 2015)

Cheyenne Mountain Resort • Colorado Springs, Colorado, 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 first two World Congresses on Integrated Computational Materials Engineering in 2011 and 2013, the 3rd World Congress on ICME (ICME 2015) will convene ICME stakeholders—including researchers, educators, and engineers—to discover the recent global advancement of ICME as an engineering discipline. Seven years after the seminal National Academies report which defined ICME as a discipline, we believe it is important to reflect on the remarkable progress that has been made and discuss where we will go in the future.

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 2015.

Warmest regards on behalf of the ICME 2015 Organizing Committee,

Warren Poole, *University of British Columbia, Canada*
Steve Christensen, *Boeing, USA*
Surya Kalidindi, *Georgia Institute of Technology, USA*
Alan Luo, *Ohio State University, USA*
Jonathan Madison, *Sandia National Laboratories, USA*
Dierk Raabe, *Max-Planck Institute, Germany*
Xin Sun, *Pacific Northwest National Laboratory, USA*

ABOUT THE CONGRESS

ORGANIZING COMMITTEE

Chair: Warren Poole, *University of British Columbia, Canada*

Steve Christensen, *Boeing, USA*
Surya Kalidindi, *Georgia Institute of Technology, USA*
Alan Luo, *Ohio State University, USA*
Jonathan Madison, *Sandia National Laboratories, USA*
Dierk Raabe, *Max-Planck Institute, Germany*
Xin Sun, *Pacific Northwest National Laboratory, USA*

INTERNATIONAL ADVISORY COMMITTEE

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Gary Purdy, *McMaster University, Canada*
Alejandro Strachan, *Purdue University, USA*
Anthony Waas, *University of Michigan, USA*
James Warren, *National Institute of Standards and Technology, USA*

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 Lower Lobby.

Sunday	5:30 p.m. to 7:30 p.m.
Monday	7:30 a.m. to 6:00 p.m.
Tuesday	7:30 a.m. to 6:00 p.m.
Wednesday	7:30 a.m. to 5:00 p.m.
Thursday	7:30 a.m. to 12:00 p.m.

Short course registration will be open from 12:00 p.m. to 1:00 p.m. on Thursday in the Lower Lobby.

Internet Access

Complimentary internet access is available for ICME 2015 attendees in some public areas of the hotel and in the guest rooms.

Technical Sessions

All oral presentations will be held in Colorado II, Colorado III, or the Amphitheater of the Cheyenne Mountain Resort. All poster presentations will be held in Colorado Ballroom I. See the Technical Program section on pages 11-44 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 $149.95 at www.wiley.com (TMS members receive a 35% discount). Approximately four 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 Colorado I.

Monday	3:00 p.m. to 4:00 p.m. 5:00 p.m. to 6:30 p.m.
Tuesday	9:00 a.m. to 11:00 a.m. 3:00 p.m. to 6:30 p.m.
Wednesday	10:00 a.m. to 12:00 p.m.

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

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MICRESS®

MICRESS® the MICRostructure Evolution Simulation Software is based on the multi-phase-field concept and is developed, maintained, and distributed by ACCESS e.V., a nonprofit research center at the RWTH Aachen University of Technology in Germany. Coupling MICRESS® to commercially available thermodynamic and mobility datasets allows for the simulation of solidification, solid state transformations, recrystallization and grain growth in technical alloy systems like steels, superalloys, aluminum/magnesium alloys and others. MICRESS® installations are currently found in Europe, US, Japan, China, India and Australia at various customers from the automotive, aerospace and steel industries, governmental research centers and universities.

Thermo-Calc Software

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 the CALPHAD method. Databases are available for steels, ferrous based slags, Ti, Al, Mg, Ni-superalloys and other materials. Software Development Kits which enable Thermo-Calc to be called directly from in-house developed software or MatLab are available. DICTRA is used for accurate simulations of diffusion in multicomponent alloys. Applications include: homogenization of alloys; microsegregation during solidification; coarsening of precipitates; and joining. TC-PRISMA is a new tool for predictions of concurrent nucleation, growth, dissolution, and coarsening of precipitate phases.

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Simpleware

Simpleware provides and develops world-leading 3D image data (CT, Micro-CT, FIB-SEM, etc.), image processing, and model generation software and services for materials science. The software can be used to easily visualise, quantify, segment, process and mesh image data for fields such as composites research, oil and gas exploration, and non-destructive evaluation. Effective material properties can also be rapidly calculated from scanned samples using homogenisation techniques, e.g., absolute permeability, elasticity, and electrical conductivity.

UES

Whether you're analyzing microstructural features in titanium alloys, correlating mechanical and thermal properties with microstructures in pitch based carbon foams, magnetic microstructures in Fe-Si alloys or porosity calculations in geometallurgy, Robo-Met.3D® (A UES Product) efficiently provides scientists new insights through visualization of materials structures in 3D.The system features customizable, precise and repeatable serial sectioning and metallographic processes with powerful image analysis. The entire process—grinding, polishing, cleaning, etching, optical microscopy, and image acquisition—is performed to your exact specifications. This high level of customizable automation enhances repeatability, and compresses data acquisition to a matter of hours.

NEW FOR 2015!

ICME TOOLS SHOWCASE

The ICME Tools Showcase is an opportunity for exhibitors and sponsors to showcase their company and products to Congress attendees. It will take place Tuesday, June 2 in Colorado II & III. The schedule is as follows:

4:00 p.m. to 4:10 p.m.	Carl Zeiss X-ray Microscopy
4:10 p.m. to 4:20 p.m.	MICRESS
4:20 p.m. to 4:30 p.m.	ESI North America
4:30 p.m. to 4:40 p.m.	Simpleware
4:40 p.m. to 4:50 p.m.	Thermo-Calc Software
4:50 p.m. to 5:00 p.m.	Materials Design Inc.

CONGRESS POLICIES

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 May 8, 2015. No refunds will be issued at the Congress. Fees and tickets are nonrefundable.

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.

Use of phones and mobile devices:
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.

Anti-Harassment
In all activities, TMS is committed to providing a professional environment free of harassment, disrespectful behavior, or other unprofessional conduct.

TMS policy prohibits conduct that is disrespectful, unprofessional, or harassing as related to any number of factors including, but not limited to, religion, ethnicity, gender, national origin or ancestry, physical or mental disability, physical appearance, medical condition, partner status, age, sexual orientation, military and veteran status, or any other characteristic protected by relevant federal, state, or local law or ordinance or regulation.

Failure to comply with this policy could lead to censure from the TMS Board of Directors, potential legal action, or other actions.

Anyone who witnesses prohibited conduct or who is the target of prohibited verbal or physical conduct should notify TMS staff member as soon as possible following the incident. It is the duty of the individual reporting the prohibited conduct to make a timely and accurate complaint so that the issue can be resolved swiftly.

Photography and Recording


TMS reserves the right to all audio and video reproduction of presentations at TMS-sponsored meetings. By registering for this meeting, all attendees acknowledge that they may be photographed by TMS personnel while at events and that those photos may be used for promotional purposes, in and on TMS publications and websites, and on social media sites.

Any 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. Attendees violating this policy may be asked to leave the session.

Antitrust Compliance
TMS complies with the antitrust laws of the United States. Attendees are encouraged to consult with their own corporate counsel for further guidance in complying with US and foreign antitrust laws and regulations.

KEEP THE ICME CONVERSATION GOING

Attend the **Implementing ICME in Industry** short course following this congress!

June 4-5, 2015 • Cheyenne Mountain Resort • Colorado Springs, Colorado, USA

For more information on the course visit the Registration Desk or visit the Short Course page of the ICME 2015 website at: http://www.tms.org/icme2015.

NETWORKING & SOCIAL EVENTS

Welcome Reception
The Welcome Reception will be held on Sunday, May 31 from 6:30 p.m. to 7:30 p.m. in the Colorado Gallery.

Poster Viewing and Reception
Poster viewing and receptions are planned for Monday, June 1 and Tuesday, June 2 from 5:00 p.m. to 6:30 p.m. following the technical sessions in Colorado I. Don't miss this great networking opportunity!

Congress Dinner
The dinner will be held on Wednesday, June 3 from 6:00 p.m. to 8:00 p.m. in Remington I & II.

ABOUT THE VENUE

Known for its breathtaking mountain views, exceptional accommodations, two restaurants and one lounge featuring Colorado fresh cuisine, a myriad of activities, and comprehensive conference facilities, the AAA Four Diamond Cheyenne Mountain Resort and Country Club offers the ultimate in Colorado vacationing. A vast array of amenities include an 18-hole championship, Pete Dye-designed golf course; five swimming pools; tennis courts; full-service fitness center; aquatics center; and a 35-acre recreation lake.

For more information,
visit www.cheyennemountain.com.

The resort offers complimentary self-parking and valet-parking in a secure outdoor lot.

TRANSPORTATION

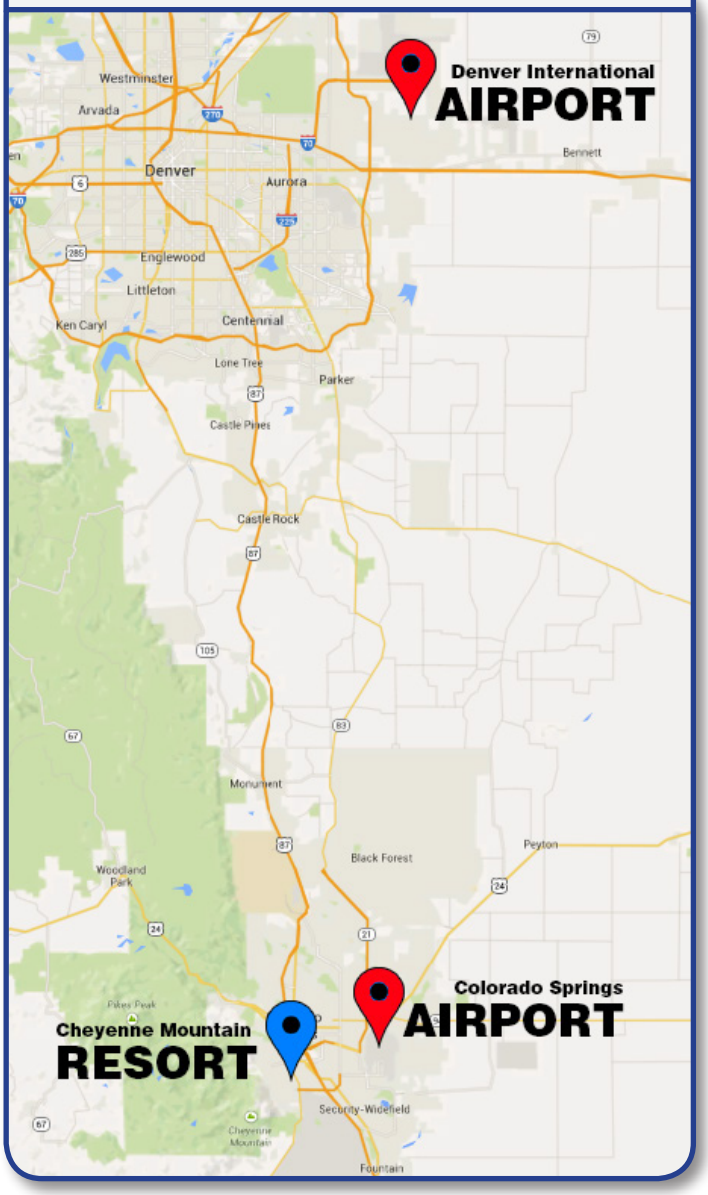
Transportation from Colorado Springs Airport (20-minute drive from resort):

- Round-Trip Shuttle Service: Approximately $40 per person
- One Way Shuttle Service: Approximately $20 per person
- Children 12 and under are free
- Shuttle transportation is provided by the resort
- Taxi Service: Approximately $26 one way
- Town Car Service: Approximately $125 one way

Hertz Rent A Car: For your convenience Hertz Rent A Car now has a service desk in the main lobby of Cheyenne Mountain Resort, offering convenient pick up and drop off right on site. The resort staff is happy to connect you to their extension or you may contact them directly at (719) 632-4000.

To make transportation arrangements, send an e-mail to cheyennemountaintransportation@benchmarkmanagement.com.

MAP OF RESORT AND AIRPORTS



TECHNICAL PROGRAM GRID

Morning Session

	Monday			Tuesday			Wednesday			Thursday
	Colorado II	Colorado III	Amphitheather	Colorado II	Colorado III	Amphitheather	Colorado II	Colorado III	Amphitheather	Colorado Ballroom II & III
8:00 AM 8:10 AM 8:20 AM 8:30 AM 8:40 AM 8:50 AM 9:00 AM 9:10 AM 9:20 AM 9:30 AM 9:40 AM 9:50 AM 10:00 AM 10:10 AM 10:20 AM 10:30 AM 10:40 AM 10:50 AM 11:00 AM 11:10 AM 11:20 AM 11:30 AM 11:40 AM 11:50 AM 12:00 PM	Plenary Session I Colorado Ballroom II & III			Applications III: Composites and Non-Ferrous	ICME Implementation and Case Studies	ICME Models, Tools and Infrastructure II	Plenary Session III Colorado Ballroom II & III			Plenary Session IV
	Break			Break			Break			Break
	Applications I: Lightweight Materials	Modeling at Different Scales I	Process and Performance Modeling I	Applications III: Composites and Non-Ferrous (continued)	ICME Implementation and Case Studies (continued)	ICME Models, Tools and Infrastructure II (continued)	Process and Performance Modeling II	Modeling at Different Scales III	ICME Models, Tools and Infrastructure III	Panel Discussion
	12:20 to 2:00 PM: Lunch on Own			12:00 to 2:00 PM: Lunch on Own			12:40 to 2:00 PM: Lunch on Own			Closing Remarks
										Congress ends

Afternoon Session

	Colorado II	Colorado III	Amphitheather	Colorado Ballroom II & III	Colorado II	Colorado III	Amphitheather
2:00 PM 2:10 PM 2:20 PM 2:30 PM 2:40 PM 2:50 PM 3:00 PM 3:10 PM 3:20 PM 3:30 PM 3:40 PM 3:50 PM 4:00 PM 4:10 PM 4:20 PM 4:30 PM 4:40 PM 4:50 PM 5:00 PM 5:10 PM 5:20 PM 5:30 PM 5:40 PM 5:50 PM 6:00 PM 6:10 PM 6:20 PM 6:30 PM	Applications II: Ferrous	Modeling at Different Scales II	ICME Models, Tools and Infrastructure I	Plenary Session II	Applications IV	Modeling at Different Scales IV	ICME Models, Tools and Infrastructure IV
	Break			Break	Break		
	Applications II: Ferrous (continued)	Modeling at Different Scales II (continued)	ICME Models, Tools and Infrastructure I (continued)	ICME Tools Showcase	Applications IV (continued)	Modeling at Different Scales IV (continued)	ICME Models, Tools and Infrastructure IV (continued)
	Poster Sesion I Colorado I			Poster Sesion II Colorado I	5:00 PM: Congress ends for the day		
	6:30 PM: Congress ends for the day			6:30 PM: Congress ends for the day			

Plenary Session I

Monday AM
June 1, 2015

Room: Colorado II & III
Location: Cheyenne Mountain Resort

8:00 AM Invited
ICME: Past, Present and Future: John Allison [1]; [1]University of Michigan

In 2008, an authoritative US National Academies panel concluded that "Integrated Computational Materials Engineering" was a new and potentially transformational discipline. That panel went on to posit that for ICME to succeed in becoming truly transformational it must be embraced as a discipline by the materials profession. The importance of ICME was demonstrated in 2011 with the inauguration of the Materials Genome Initiative. This talk will provide a perspective on what has transpired since 2008 and on the current state of ICME. I will also provide thoughts on the challenges and opportunities that lie before us as well as a prognosis for the future.

8:30 AM Invited
ICME: A Perspective on the Progress and Challenges: *Tresa Pollock*[1]; [1]University of California Santa Barbara

The design and implementation of new materials into advanced engineering systems has long been recognized as challenged by the speed of design and the high materials development costs. The confluence of advanced computation, new capabilities for data analytics and rapid characterization has paved the way for national ICME efforts, including the Materials Genome Initiative. Recent examples of the impact of the ICME approach on materials development will be reviewed along with challenges for future integration of emerging tools and approaches.

9:00 AM Question and Answer Period

9:20 AM Invited
Materials Genomics: From CALPHAD 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, while the DARPA-AIM initiative has broadened computational materials engineering to address acceleration of the full materials development and qualification cycle. Integration with the full suite of fundamental databases and models has demonstrated the historic milestone of greatly accelerated flight qualification for two aircraft landing gear steels. In support of the national MGI, the new NIST-sponsored CHiMaD Center for Hierarchical Materials Design expands the scope of genomic materials design across materials classes.

9:40 AM Invited
Multiscale Modeling of Phase Transformations in High-performance Steels: *Matthias Militzer*[1]; [1]The University of British Columbia

The austenite-ferrite transformation is a key metallurgical tool to manufacture high-performance steels with improved properties. Significant progress has been made in developing knowledge-based process models for the steel industry. The predictive capabilities of these models are limited as a number of empirical parameters are required to describe microstructure evolution and resulting properties. Modeling across different length and time scales offers tremendous opportunities to develop next-generation process models with enhanced predictive capabilities for the design of steel chemistries and processing routes. The status and challenges of the proposed multiscale approach will be discussed for microstructure evolution in advanced low-carbon steels. In particular, the linkage between atomistic simulations, phase-field modeling and conventional diffusion models will be illustrated for the effect of alloying elements on the austenite-ferrite transformation. The proposed model approach will be validated with experimental observations for continuous cooling transformation in commercial steels.

10:00 AM Break

Applications I: Lightweight Materials

Monday AM
June 1, 2015

Room: Colorado II
Location: Cheyenne Mountain Resort

10:20 AM
Experiments and Modeling of Three-dimensional Dendritic Morphology of Magnesium Alloy: Manhong Yang[1]; Zhipeng Guo[1]; *Shou-Mei Xiong*[1]; [1]Tsinghua University

Magnesium alloys are one of the lightest structural materials. The mechanical properties of magnesium alloys are often determined by the dendritic microstructures. With hexagonal close-packed (HCP) structure, the preferred growth orientation of magnesium alloys was supposed to be <11$\bar{2}$0> all the time, and different three-dimensional growth models of magnesium alloys were proposed. However, these growth models of magnesium alloys were divergent and not yet generally accepted. Recently, Mg-20wt.%Y alloys with different solidification conditions were studied by synchrotron X-ray tomography to establish the three-dimensional dendritic morphology of magnesium alloy. The dendritic microstructures of a-Mg (Y) were reconstructed by data processing technology. From the reconstructed results, we found that the a-Mg (Y) dendrites grow along eighteen branches with six branches along <11$\bar{2}$0> orientation in the {0001} basal plane, and twelve branches along <11$\bar{2}$x> orientation in non-basal plane. Combined with the three-dimensional dendritic morphology of a-Mg (Y), a numerical model based on cellular automaton method was developed to simulate the dendritic growth of magnesium alloys. The growth kinetics was calculated through the complete solution of transport equations and a three-dimensional anisotropy growth model was constructed with cubic cellular automaton cells. Simulated results show that three-dimensional dendrites also have eighteen branches, which is the same with the reconstructed morphology by synchrotron X-ray tomography. Meanwhile, the three-dimensional simulated results were also compared and validated with two-dimensional microstructures obtained by scanning electronic microscope. Both the experimental and simulated results offer a deep insight into the dendritic growth evolution of magnesium alloys during solidification.

10:40 AM
Sensitization Effects on the Fracture and Fatigue Crack Growth Behavior of Al-Mg Alloys: *Mohsen Seifi*[1]; Hao Jiang[1]; Bo Li[1]; John Lewandowski[1]; [1]Case Western Reserve University

Al-Mg 5xxx alloys are desirable in a wide array of structural applications that require a weldable alloy with good corrosion resistance. However, significant changes in the mechanical properties have been shown to occur after long term thermal exposures (e.g. 1000's hrs). Commercially available 5xxx alloy plates have been thermally exposed to various low and intermediate temperatures for up to 20,000 hrs. Significant changes to the hardness, tension and fatigue crack growth behavior have been observed after such exposures. In particular, longitudinal splitting in the short-transverse (ST) direction has been exhibited during fatigue after sufficient time and temperature exposure combinations. These splits happen in certain orientations and their appearance depends on the testing orientation. Finite Element simulations of three point bending tests on the 5xxx alloy specimens treated in different conditions are employed to obtain the full stress field in the materials in order to calculate the stresses in various directions and orientations. The computational results are integrated with experimental measurements to identify the critical stress state for the evolution of splitting in fatigue and understand the competition between fatigue crack propagation and ST splitting.

11:00 AM

Computer Simulations of Mg/Al Cladding Process by Twin-roll Casting: *Jong-Jin Park*[1]; [1]Hongik University

Sheets of magnesium alloys are expected to be used in the automotive industry because of their good physical properties. However, poor corrosion resistance is one of drawbacks to be resolved. One of methods to improve the corrosion resistance of the sheets is to clad a layer of a material with good corrosion resistance. In the present investigation, computer simulations of a cladding process by a vertical twin-roll casting were performed. In the process, the melt of an aluminum alloy is supplied to both sides of the surface of a magnesium alloy sheet in a twin-roll caster, and the rolls cool the melt and control the thickness of the cladded sheet. Important parameters in this process are initial temperatures of the melt and the magnesium sheet, roll speed and roll contact angle. If these parameters are improperly selected, the process is unable to function or the cladded sheet is defective. Through computer simulations, required roll separating force and roll torque were found and the process can be evaluated in view of capacities of the twin-roll caster. Also the complex thermo-mechanical phenomenon during the process including melt flow, cooling, solidification and rolling was analyzed to provide information on various aspects of final properties. The temperature distribution at the interface was also found which is critical for a sound interfacial bonding. Details of findings will be presented and discussed.

11:20 AM

An Integrated Simulation Tool for Novel Mg and Al Alloy Design: *Manas Paliwal*[1]; In-Ho Jung[1]; [1]McGill University

The design of automotive components using light alloys such as Mg and Al has attracted great attention of automotive industry for increasing fuel efficiency and reducing CO2 emission. Although many automotive components made of steel have been tested for the replacement with Mg and Al alloys, the actual usage of light alloys in vehicles is still limited. One of the reasons limiting their applications is inferior mechanical properties compared to steel. In order to improve the mechanical properties of light alloy, the microstructure of the alloy should be tightly controlled at every processing stage commencing with casting followed by heat treatment and solution treatments.Thermodynamic and kinetic knowledge is indispensable to understand the microstructural development of alloys. In order to keep pace with Mg and Al alloy developments, light alloy thermodynamic database has been developed by the FactSage group (www.factsage.com) over the last 10 years. Recently, solidification, diffusion and precipitation simulation models for Mg and Al alloys have been also developed to predict the evolution of as cast and homogenized microstructure of Mg and Al alloys. Critical experiments to evaluate/improve thermodynamic database and kinetic simulations for Mg and Al alloys have been simultaneously carried out. In the present study, the current state of development of the kinetic simulation tools for solidification and homogenization process will be presented along with several application examples pertaining to commercial Mg and Al alloys.

11:40 AM

A Phase Field Simulation of the Recrystallization Process after High Temperature Deformations of Al-Mn-Fe-Si (AA3XXX) Alloys: *Jingqi Chen*[1]; Benqiang Zhu[1]; Warren Poole[1]; [1]The University of British Columbia

In order to study the recrystallization mechanisms after high temperature extrusion, two types of Al-Mn-Fe-Si (AA3XXX) alloys, one with a high density of dispersoids and the other without dispersoids, were extruded at high temperatures, i.e. ˜ 400 °C. Based on the experimental observations from axisymmetric extrusions, the recrystallization process is considered to be achieved by the mechanism of the continuous subgrain coarsening. The reason that <001> grains (<001> orientations // the extrusion direction) dominate recrystallization microstructure is considered to be due to their high fractions of the grain boundaries showing misorientations of 8 to 15 ° and the long-range misorientation gradients formed inside. In order to confirm such hypothesis, a 2D phase field model has been developed to describe the subgrain coarsening behaviour, where the mobility and energy of the boundary is dependent on its misorientation. According to the phase field study, <001> grains consume other orientated grains and finally dominate the recrystallization microstructure. On the other hand, when different values of Zener drag from dispersoids were introduced into the simulations, the final subgrain sizes predicted by the phase field model were similar with the experimental observations. Furthermore, the phase field method was also applied to a different strain path, i.e. plane strain deformation. In plane strain deformation, the deformation textures and deformed state are different. Using these initial condition, the phase field model has then been used to predict recrystallization behaviour.

12:00 PM Lunch Break

Modeling at Different Scales I

Monday AM
June 1, 2015

Room: Colorado III
Location: Cheyenne Mountain Resort

10:20 AM

Investigating Dislocation-vacancy Interactions at the Atomic Scale: *Lucas Hale*[1]; Chandler Becker[1]; Zachary Trautt[1]; Jonathan Zimmerman[2]; [1]National Institute of Standards and Technology; [2]Sandia National Laboratories

The atomic nature of dislocation-vacancy interactions is investigated using classical interatomic potentials. In metals and semiconductors, plasticity is predominantly controlled by dislocation motion. The ease at which a dislocation can move through a given material is greatly influenced by the presence of other defects. Obtaining a better understanding of these interactions can help improve mesoscale and continuum scale plasticity models by accounting for atomic scale behaviors. A framework for studying dislocation core structures and slip behaviors is being developed in Python to be made freely available as part of the NIST Interatomic Potentials Repository Project. Using this framework, simulations are performed that investigate how the presence of vacancies influences the dislocation core structure and energy, as well as the static and dynamic characteristics associated with dislocation slip. Statistical analysis of the accumulated results will facilitate the creation of new mesoscale models capable of capturing how vacancy concentrations influence dislocation mobility.

10:40 AM

A Molecular Dynamics Simulation Mechanism with Imprecise Interatomic Potentials: *Anh Tran*[1]; Yan Wang[1]; [1]Georgia Institute of Technology

In molecular dynamics (MD) simulation, atomic interaction is characterized by the interatomic potential energy as the input of simulation models. The interatomic potentials are derived experimentally or from first-principles calculations. Therefore they are inherently imprecise because of the measurement or model-form errors. In this work, a reliable molecular dynamics (R-MD) mechanism is developed to extend the predictive capability of MD given the input uncertainty. In R-MD, the locations and velocities of particles are not assumed to be precisely known as in traditional MD. Instead, they are represented as intervals in order to capture the input uncertainty associated with the atomistic model. The advantage of the new mechanism is the significant reduction of computational cost from traditional sensitivity analysis when assessing the effects of input uncertainty. A formalism of generalized interval is incorporated in R-MD, as an intrusive uncertainty quantification method, to model the propagation of uncertainty during the simulation. Error generating functions associated interatomic potentials are developed to capture the bounds of input variations.

11:00 AM

Multiscale Modeling of Thermal Protection Materials I: Atomistic Modeling of Constituent Properties: *John Lawson*[1]; Joshua Monk[1]; Charles Bauschlicher[1]; Steven Arnold[2]; Pappu Murthy[2]; Brett Bednarcyk[2]; [1]NASA Ames Research Center; [2]NASA Glenn Research Center

Thermal protection materials for use as heat shields for space vehicles entering planetary atmospheres experience some of the most extreme operating environments known. These materials are typically ablative composites consisting of a carbon fiber based reinforcement with a phenolic polymer resin matrix. These materials are necessarily multi-functional and multiscale systems with very high performance requirements across a range of thermal, mechanical, and chemical properties. This talk is the first of two contributions on multiscale modeling of this important class of materials. In part I, we present results from detailed atomistic simulations of the phenolic resin and carbon fiber constituents. In part II (Arnold et al), we use these atomistically informed constituent properties as input parameters for micromechanical computations of the effective composite level properties. Molecular dynamics simulations of bulk phenolic systems were performed to obtain thermal and mechanical properties as a function of the degree of cross-linking, the chemical structure of the phenolic chains and also temperature. Atomistic models were generated by a procedure which approximately mimics resin processing where cross-links were systematically introduced between chains resulting in full three dimensional thermoset networks. Using these models, a range of properties were computed including glass transition temperature, coefficient of thermal expansion, density, elastic and shear moduli and thermal conductivity. Simulation results were validated against experimental data and excellent agreement was found. These results give the detailed relationship between the chemical structure of the resin and constituent level properties, pointing the way to chemical design of improved high performance resins.

11:20 AM

First-principles Study of Interface between Iron and Precipitate: *Hideaki Sawada*[1]; Shunsuke Taniguchi[1]; Kazuto Kawakami[1]; Taisuke Ozaki[2]; [1]Nippon Steel & Sumitomo Metal Corporation; [2]The University of Tokyo

In steel there are some precipitates which undergo transition from coherent to semi-coherent precipitate during growth. Semi-coherent precipitates can provide much different performance than coherent precipitates for example strength, hydrogen trap and so on. The performance of steel can be improved by the proper usage of coherent and semi-coherent precipitates. Therefore, it is important to know the size where the precipitate undergoes the transition from coherent to semi-coherent state. In this study NaCl type compounds, NbC and TiC, are chosen as precipitate. It is necessary to obtain the interface and strain energies due to precipitate in order to know the transition size from coherent to semi-coherent precipitate. The interface energy is calculated by the use of the O(N) Krylov-subspace method of first-principles calculation1). The strain energy is estimated by the classical molecular dynamics simulation. The calculated interface and strain energies for TiC indicate that the transition size from coherent to semi-coherent precipitate is about 2.3 nm. The precipitate size dependence of interaction force on a dislocation due to precipitate obstacle changes around 2.5 nm2). If the change in the precipitate size dependence of interaction force is attributed to the transition from coherent to semi-coherent precipitate, this calculation method gives fairly accurate value.

11:40 AM

Prediction of Microstructure and Mechanical Properties in Aluminum High Pressure Die Castings after Heat Treatment: *Jianzheng Guo*[1]; Sam Scott[2]; Weisheng Cao[3]; [1]ESI US R&D; [2]ESI NA; [3]Computherm LLC

With the current transportation industry push towards vehicle lightweighting, materials and alloys that were previously thought unsuitable for structural components are gaining a renewed interest in concert with new manufacturing technology that makes these materials valid and popular choices in applications requiring strength. This industry movement generates a need to better understand the material property history of the component through the manufacturing process, and ideally use that information in simulations of component performance. A numerical model is being developed for the calculation of the microstructure and mechanical properties of aluminum high pressure die castings after heat treatment. Based on the alloy chemical composition, solidification and heat treatment processing, the model predicts the microstructure, potential defects, and mechanical properties in the frame work of ICME approach. The simulation of the different manufacturing process stages is integrated such that the resultant microstructure of the previous event is used as the initial condition of the following event, ensuring the tracking of the component history while maintaining a high level of accuracy across these metallurgical stages. Such integration is helpful to understand the effects of alloy chemistry and processing conditions with their relationship to microstructure, defect formation, and the final mechanical properties from solidification through heat treatment. In this paper an A383 alloy is selected as an example to study the microstructure and mechanical properties evolution through the process of casting to heat treatment numerically, with a focus on a casting process with high cooling rate, such as high pressure die casting.

12:00 PM

Multiscale Modeling of Thermal Protection Materials II: Micromechanical Modeling of Composite Performance: *Steven Arnold*[1]; Pappu Murthy[1]; Brett Bednarcyk[1]; John Lawson[1]; Charles Bauschlicher[1]; Joshua Monk[1]; [1]NASA

This talk is the second of two contributions on multiscale modeling of thermal protection materials for space vehicles (also see Lawson et al). In part I, atomistic simulations were used to derive constituent properties, while here; we perform micromechanical computations to obtain composite level effective properties. A new class of ablative materials based on woven carbon reinforcement is considered. An integrated computational approach that captures the effect of different woven architectures along with different materials constituent can result in a potentially powerful design tool to navigate the large design space for this important class of materials.In the case of woven ablative composites, significant variations in the microstructure of the composite exist and their impact on thermal and deformation response needs to be assessed. Several examples of the variations are changes in the weave, fiber tow shape, fiber packing structure within tows, and voids within and between tows. The effects of these architectural parameters and constituent material properties will be captured at the appropriate length scale. The Multiscale Generalized Method of Cells methodology is used to determine the overall effective composite properties, deformation response, and failure under tensile loading conditions for 2D woven composite materials. Linkage to processing and the atomistic scale is achieved through molecular dynamics modeling at the constituent level. These "atomistically informed" constituent properties will in turn affect the overall composite response through the associated micromechanical modeling. Validation of the present multiscale modeling approach is achieved through comparison with previously obtained experimental composite results.

12:20 PM Lunch Break

Process and Performance Modeling I

Monday AM
June 1, 2015

Room: Amphitheater
Location: Cheyenne Mountain Resort

10:20 AM

Direct Numerical Simulations in Solid Mechanics for Understanding the Engineering-scale Effects of Microstructure: *Joseph Bishop*[1]; John Emery[1]; [1]Sandia National Laboratories

A fundamental challenge for the quantification of uncertainty in solid mechanics is understanding how microstructural material variability is manifested at the macroscale. This understanding is particularly important if the assumption of scale separation inherent in homogenization theory is no longer appropriate, e.g., when the characteristic length of the microstructure is comparable to structural feature sizes. This loss of scale separation is particularly apparent in additive microstructures. In order to understand how microstructural material variability is manifested at the engineering scale, and to understand the limitations of homogenization theory, we perform an ensemble of Direct Numerical Simulations (DNS) in which microstructures are embedded directly within engineering scale structures. High-performance computing resources are used to model the structure with a finite element mesh of sufficient refinement to also resolve the microstructure. Crystal-plasticity models are used to represent the grain-scale physics. The DNS simulations are compared with conventional simulations that use material properties obtained from homogenization theory. Quantitative comparisons are made in both the elastic and elastic-plastic regimes.

10:40 AM

Meso-Scale Predictions of Laser-Weld Microstructure via Kinetic Monte-Carlo Simulation: *Jonathan Madison*[1]; Efrain Hernandez[2]; Veena Tikare[1]; [1]Sandia National Laboratories; [2]University of Michigan

Using Sandia National Laboratories' kinetic monte-carlo simulator known as SPPARKS (Stochastic Parallel PARticle Kinetic Simulator), a user-routine has been created to produce meso-scale predictions of grain structure within the vicinity of a moving heat-source. The simulation is chiefly applicable to a variety of welding and some additive manufacturing applications while providing qualitative agreement for both grain size and grain morphology by incorporating heat source shape, energy profile and travel speed . The fundamental mechanisms of the model will be discussed and a comparison of the model with experiments will be presented.Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000

11:00 AM

ICME Application in Optimizing Welding and Thermal-Forming Processes: *Yu-Ping Yang*[1]; Hyunok Kim[1]; Bill Mohr[1]; Harvey Castner[1]; TD Huang[2]; Dennis Fanguy[3]; [1]EWI; [2]Ingalls Shipbuilding; [3]Bollinger Shipyard

Integrated computational materials engineering (ICME) is an emerging discipline that can accelerate product development and unify design and manufacturing. This paper summarizes the ICME applications for optimizing welding and thermal-forming processes. In the first application, numerical

analyses were conducted to control weld distortion by using intermittent welding to replace full-length double-sided fillet welds and adapting new low heat-input processes such as hybrid laser-arc welding process. In the second application, an existing software tool was validated and applied to automate thermal plate forming, a process which has been extensively used in the shipbuilding industry to form curved plates for several decades.

11:20 AM

Resolving the Evolution of Pore Structures in 304-L Laser Welds Through Remeshing and Mapping of Internal State Variables: *James Foulk*[1]; [1]Sandia National Laboratories

The failure of partial-penetration Nd:YAG laser welds in 304-L stainless steel have been investigated through the direct incorporation of pore structures at the specimen level. Micro-computed tomography (μCT) is employed to characterize multiple weld schedules and develop idealized representations of the size, shape, and spacing of the pores. Pore growth and the subsequent necking are natural outcomes of the simulation. The large deformations between pores require a robust mapping scheme for the remeshing and mapping of internal state variables. We employ higher-order tetrahedral elements to resolve strong gradients and ease the burden of discretizing complex and evolving pore structures. Through our ability to idealize, resolve, and evolve pore structures, we can investigate the performance of candidate weld schedules. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

11:40 AM

Manufacturing and Evaluation of High Entropy Alloys: Joseph Licavoli[1]; *Paul Jablonski*[1]; Michael Gao[1]; Jeff Hawk[1]; [1]Department of Energy

High entropy alloys (HEA) have generated interest in recent years due to their unique positioning within the alloy world. By incorporating a number of elements in high proportion they have high configurational entropy which leads to interesting and useful properties such as enhanced oxidation resistance and strength. In the past, researchers have relied on a simple calculation to determine this configurational entropy which results in equiatomic compositions. Here we take an alternate approach where we use the CALPHAD method to calculate the optimum (highest) entropy for a system of elements. Interestingly, we have found that this leads to an alternate alloy formulation. We will compare equiatomic alloys to the same system of elements formulated with an optimum entropy. These alloys are made as large scale ingots in our lab using detailed process control which is easily transferred to commercial production. Our preferred approach is to employ induction melting to form a fully alloyed structure followed by application of a computationally optimized homogenization treatment which is followed by hot working. The resulting structure is fully wrought and comparable to manufacture on the commercial scale. We will present our alloys and microstructural control along with resulting representative properties such as tensile and oxidation resistance and make comparisons between the formulations. A discussion regarding alternative approaches to material fabrication and the impact on resulting properties will also be presented.

12:00 PM

Computational Evaluation of Coatings and Surface Treatments in Prevention of Fretting Fatigue: *Xiawa Wu*[1]; Nathan Bolander[1]; Behrooz Jalalahmadi[1]; [1]Sentient Science

Fretting fatigue is one of the safety concerns in rotorcraft applications. Fretting is a wear phenomena that can reduce the fatigue strength of components by more than 50%. Under fretting conditions, microcrack initiates and propagates without easy detection due to its microscale origin which raises the need to seek a computational tool to model the material behavior at micro level and predict macro level component life. Sentient develops a microstructure-based component life prediction (CLP) tool through Integrated Computational Materials Engineering (ICME) modeling and simulation to address this issue and simulates and evaluates fretting fatigue on splines. The experimentally validated results indicate that surface condition plays an important role in fatigue cracks in fretting regions. Coatings and processing treatments can be used to prevent the fretting fatigue through optimizing surface and subsurface stress distribution, reducing relative displacement between two contacting surfaces and improving coefficient of friction. Sentient extends CLP to include the capability of coating modeling and evaluates the effect of different coating materials, their abilities to prevent fretting fatigue failures and extend component life. The advantage of applying this computational method is a in-depth understanding of coating effects and a reduction of the number of experimental deposition and characterization. Coating material type, microstructure, thickness, bonding strength to the substrate and surface treatment are considered and simulated in the model, which can guide experimental designs, reduce the non-productive trials and provide optimum results.

12:20 PM Lunch Break

Applications II: Ferrous

Monday PM
June 1, 2015

Room: Colorado II
Location: Cheyenne Mountain Resort

2:00 PM

Development of Q&P Steels with Improved Performance based on Microstructure-based Finite Element Modeling Method: *Kyoo Sil Choi*[1]; Xiaohua Hu[1]; Xin Sun[1]; Mark Taylor[2]; Emmanuel DeMoor[2]; John Speer[2]; David Matlock[2]; [1]Pacific Northwest National Laboratory; [2]Colorado School of Mines

3rd generation AHSS (advanced-high-strength-steels) concepts are pursued vigorously to identify lower alloy steels which achieve ultra-high-strength and good formability for implementation in automotive production. A possible strategy to achieve the property and cost requirements of the 3rd generation AHSS is to improve martensitic steels with enhanced retained austenite levels (i.e., Q&P (quenching-and-partitioning) steel). In this work, a microstructure-based finite element modeling method was adopted in investigating the effects of material parameters of the constituent phases on the macroscopic tensile behavior of Q&P steel, and new Q&P heat-treating parameters were then devised based on the modeling results to produce Q&P steels with improved performance. A model Q&P steel was first produced and various experiments were performed for material characterization. Actual microstructure-based model was generated based on the information from the tests, and the material properties for the constituents in the model were estimated based on in-situ HEXRD (high-energy-X-ray-diffraction) test. Influence of various material parameters of the constituents on the macroscopic behavior was then investigated. Based on the observation of the respective influence of constituent material parameters, a computational material design was also performed for performance improvement. The modeling results indicate that various material parameters need to be concurrently adjusted in a cohesive way for the performance improvement of Q&P steels. In summary, higher austenite stability, less strength difference between the phases, and higher hardening exponents of the phases are generally beneficial for performance improvement. Based on the information from the modeling works, new Q&P steels with improved performance were then produced.

2:20 PM
ICME Towards Improved Understanding of Bainite in 100Cr6: *Wenwen Song*[1]; Wolfgang Bleck[1]; Ulrich Prahl[1]; [1]RWTH Aachen University

In the design of high strength steels bainite structures gain importance because of their excellent balance of strength and toughness. However, Bainite still remains the least understood austenite decomposition reaction. Following the philosophy of Integrated Computational Materials Engineering (ICME) we combine various simulation and advanced characterization approaches at different length scales in order to improve the scientific analysis of this solid phase transformation with combined chemical-diffusive and mechanical contribution. In the present work, bainite transformation in 100Cr6 steel with nano-sized cementite (θ) precipitation within bainitic ferrite (aB) is analyzed. The bainite transformation was introduced and investigated by TEM, atom probe tomography (APT), phase-field simulations and ab initio calculations. APT shows that in lower bainite isothermally held at 260 °C both e and θ precipitate adopting plate-like shapes and precipitate under para equilibrium mode. With the help of atom probe concentration data input and para-equilibrium phase diagram calculation using ThermoCalc software, microstructure evolution and phase transformation kinetics during isothermal bainite formation was predicted by means of phase field simulation. To simulate the very fine cementite, ultra-small grid spacing, i.e. 2 nm, is applied in the simulation. A faceted model has been coupled in the simulation for both bainitic ferrite (aB) and cementite (θ) growth. APT showed the high amount of carbon trapped within bainitic ferrite. It is of significant importance to take into account both carbon partitioning and carbon trapping within bainite ferrite in bainite transformation simulations. Carbon redistribution across γ/aB and aB/θ phase boundaries during bainite transformation is further discussed.

2:40 PM
ICME Approaches to Design Advanced Steels: Application to Transformation Induced Plasticity and Alumina Forming Stainless Steels: *Raymundo Arroyave*[1]; Shengyen Li[1]; Taymaz Jozaghi[1]; Chung J. Wang[1]; Shujuan Wang[1]; Ibrahim Karaman[1]; [1]Texas A & M University

In this talk, we will discuss some examples in which computational thermodynamics and kinetics have been used in combination with computational optimization strategies have been used to optimize alloy performance under a wide range of constraints. First, we will discuss our recent work on Transformation Induced Plasticity Steels, where alloy and processing parameters constitute the degrees of freedom to be optimized in order to attain phase constitutions that result in superior combined strength and ductility. Experiments and computations are used to establish alloy/processing-microstructure-performance relations and the latter are used in the optimization scheme. A second example will be our more recent work on the development of alumina-forming, twinnable stainless steel alloys. In this case, thermodynamic and kinetic-based criteria are used to determine the conditions necessary for the formation of stable alumina protective layers as well as the the ability of the alloy to form deformation twins.

3:00 PM
Steel – Ab initio: Quantum Mechanics Guided Design of New Fe-Based Materials: *Wenwen Song*[1]; Ulrich Prahl[1]; Wolfgang Bleck[1]; [1]RWTH Aachen University

This contribution reports the results of the collaborative research unit SFB 761 “Steel - ab initio”, a cooperative project between RWTH Aachen University and the Max-Planck-Institute for Iron Research in Düsseldorf (MPIE) financed by the German Research Foundation (DFG). For the first time, in a structural measure it is exploited how ab initio approaches may lead to a detailed understanding and thus to a specific improvement of the design process for a structural steel. Here, 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 new type of structural materials based on Fe-Mn-C and Fe-Mn-Al-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: a) development of a new method for material- and process-development based on ab initio calculations; b) design of a new class of structural materials with extraordinary property combinations; c) acceleration of development time and reduction of experimental efforts and complexity for material- and process-development. In the present work, the general concept of the new design concept is presented together with some exemplarily results showing the advantage of this combined scale bridging approach.

3:20 PM Break

3:40 PM
Development of an ICME Framework for Steel Ingot Processing: *Stephane Forsik*[1]; Jeffrey Yanke[1]; Richard Smith[1]; Mario Epler[1]; [1]Carpenter Technology Corporation

Premium steels are often manufactured by vacuum induction melting (VIM) followed by vacuum arc remelting (VAR). During solidification, a dendritic structure develops and alloying elements with a partition coefficient lower than one partition to the liquid, producing a microsegregated structure that must be homogenized. The temperature and duration of the homogenization are determined by the severity of the microsegregation, the secondary dendritic arm spacing (SDAS) and the dimensions of the ingot, and must take into account industrial and economic constraints. The temperature is crucial because it must be high enough to rapidly diffuse slow-moving elements over long distances but low enough to avoid any risk of incipient melting. Various computational techniques used in an ICME framework can model the microstructure development and simulate the effects of the homogenization on microsegregation. Specifically, VAR modeling can predict the local solidification time and give location-specific cooling rates used to predict the SDAS. CALPHAD-based methods can calculate the microsegregation profiles (Thermo-Calc) and simulate diffusion (Dictra). Given this data, and accounting for heat transfer effects, an efficient homogenization cycle avoiding incipient melting is determined through modeling.An ICME framework was applied to a VIM-VAR cast ingot of M50, a tool steel, to determine the appropriate homogenization cycle. The microstructure parameters were predicted and a homogenization cycle that is compatible with industrial production was calculated. Experimental validation was shown for a 400-lb (181.4 kg) lab scale VIM-VAR ingot from which samples were extracted and subjected to various homogenization heat treatments.

4:00 PM
Finite Element Modeling for Plymouth Tube Processing with Internal State Variables: *Heechen Cho*[1]; Youssef Hammi[1]; Mark Horstemeyer[1]; [1]Mississippi State University

In order to model the sequential processing steps of materials, the history dependence of the stresses, strains, and microstructural content must be included to capture high fidelity solutions. The history dependent numerical solutions for deformation processes of a material can give critical information that helps to understand how the target material behaves in specific mechanical or thermo-mechanical conditions. In this study, history dependent numerical simulations were performed to model major tubing processes that have been used in manufacturing. In order to implement the history dependent model, Internal State Variables (ISV) Plasticity-Damage (DMG) model that have been developed at Sandia National Labs and Mississippi State University was employed for a low carbon steel AISI 1010 which is actually used in a tube manufacturing company. Even though the model is performed at the structural scale, the history variables (internal state variables) which are driven by microstructural changes, e.g., dislocation density, were tracked through the whole sequences, and the history model captured most of real thermal and mechanical behaviors of the target material. Besides, once the internal state variables were extracted from the simulation, the model showed critical deformation histories that one could not notice with the naked eye and must be considered for design of the tubing processes.

4:20 PM
Ab-initio Calculation of Solute Effects on Austenite Grain Boundary Properties in Steel: *Michael Hoerner*[1]; Mark Eberhart[1]; John Speer[1]; [1]Colorado School of Mines

Ab-initio density functional theory calculations have been performed to determine the effect of solutes including Cr, Ni, Mo, and C on the boundary energy and atomic migration activation energies for a variety of coincident site lattice grain boundaries of FCC iron (austenite). The boundaries investigated were of both tilt and mixed character and both symmetric and asymmetric boundary planes were investigated. Boundary energies were determined for

boundaries in pure Fe and for boundaries with single solute atoms at multiple sites per boundary. Activation energies were determined for atomic motions that are predicted by molecular dynamics simulations at select boundaries in the literature. The results are compared to Arrhenius type equations developed from experimental work in the literature and used to develop a mechanistic model for the effects of solutes on boundary mobility based upon the thermodynamic and kinetic effects of solutes at austenite grain boundaries. The predictive capabilities of the model are evaluated and areas for future work are identified. This work provides a new framework for understanding the effects of solutes on atomic scale grain boundary migration mechanisms and solute drag effects on boundaries.

Modeling at Different Scales II

Monday PM
June 1, 2015

Room: Colorado III
Location: Cheyenne Mountain Resort

2:00 PM

Multi-scale Simulation to Help Predict Morphology Generated by Reaction Induced Phase Separation: *Dominic Wadkin-Snaith*[1]; Matthew Jackson[1]; [1]Cytec

Toughening of thermoset composite matrix resins can be accomplished by the incorporation of thermoplastic polymer in the un-cured thermoset resin. Cure can then result in separation into a thermoplastic- rich and thermoset-rich phase. This phenomena is referred to as Reaction Induced Phase Separation. The toughness of the resin is then strongly dependent on the phase morphology. Bennett's acceptance ratio has been used to calculate the Flory interaction parameter as a function of temperature and the cross link density of the thermoset which increases during cure. This interaction parameter is used to determine the degree of cure at which any phase separation would occur. With a value for the boundary gradient coefficient, concentration dynamics can be simulated using the Cahn-Hilliard equation. This allows exploration of the effect of cure cycle on morphology.

2:20 PM

Virtual Testing of Polycrystalline Ni-based Superalloys: From Single Crystals to Design Allowables: Aitor Cuadrado[1]; Bin Gan[1]; Javier Segurado[2]; Jon Mikel Molina-Aldareguía[1]; *Javier LLorca*[2]; [1]IMDEA Materials Institute; [2]Polytechnic University of Madrid & IMDEA Materials Institute

A novel multiscale modeling approach is presented for predicting the mechanical properties of wrought or cast polycrystalline Ni-based superalloys. The single crystal properties are obtained from compression tests carried out in micropillars obtained by FIB machining with different orientation (single and multiple slip) from the polycrystalline sample. Micropillar tests at different temperatures and strain rates are used to determine the parameters of both phenomenological and physically-based single crystal plasticity models. In parallel, a three-dimensional representative volume (RVE) of the polycrystalline microstructure is built using Voronoi tessellation. The initial distribution of points for the Voronoi tessellation is optimized by means of a Monte Carlo algorithm to fit the experimental grain size distribution of the polycrystal. The mechanical behavior of the polycrystal is determined by means of the finite element analysis of the RVE with periodic boundary conditions. The single crystal plasticity models obtained from the micropillar compression tests are used as the constitutive equation of each grain. In addition, cohesive elements are introduced between the grains to simulate grain boundary sliding. The results of the multiscale modeling strategy are compared with experimental results of the tensile and compressive strength wrought and cast polycrystalline IN718 as a function of temperature. The potential of this approach to carry out virtual testing of polycrystalline Ni-based superalloys within the framework of integrated computational materials engineering is discussed.

2:40 PM

Connecting Metallic Glass Mechanics with Its Deformation Physics via a Shear Transformation Zone Dynamics Model: *Lin Li*[1]; [1]University of Alabama

Metallic glasses exhibit a rich diversity of deformation behaviors depending upon thermal and mechanical loading conditions. The details of how the diverse behaviors are connected pertain to the underlying deformation mechanism of local shear shuffling in the amorphous glass structure. In the spirit of the original works on shear transformation zone (STZ) by Argon and free volume by Spaepen, we develop a meso-scale STZ-dynamics model, which adopts the STZ as a fundamental deformation unit and as well incorporates the free volume as an internal structure-related variable, and further employ this model to investigate the interplay of glass deformation and free volume evolution. The STZ-dynamics model coarse-grains an amorphous collection of atoms into an ensemble of STZs on a mesh, and evolves via two competing processes: STZ activation that creates the free volume, vs. diffusive rearrangement that annihilates it. A kinetic Monte Carlo algorithm is employed to determine the activation sequence, and finite element analysis is performed to calculate the local stress, strain and free volume redistribution after each activation event. Overall, the model is able to capture the diverse deformation behaviors of metallic glasses, including high-temperature homogeneous flow, and low-temperature strain localization into shear bands. In this talk, the development of the model as well as its applications to metallic glass processing and deformation will be discussed.

3:00 PM

Multi-scale Modelling of Interfacial Energies on the Nanoscale: From Analytical to Quantum Mechanical: *Wenwu Xu*[1]; Andrew Horsfield[2]; Peter Lee[1]; [1]The University of Manchester; [2]Imperial College London

Accurate determination of interfacial energies is critical to a proper understanding of the properties of bonded materials; this is especially so for nanomaterials having a large volume fraction associated with interfaces. Yet, in spite of this importance, reliable methods to measure interfacial energies of nanomaterials remain elusive. Experimental effort to measure interfacial energies is mostly focused on interfaces where liquid and/or gas is presented, such as solid/liquid and liquid/gas interfaces. Direct experimental measurement of solid state interfacial energy on the nanoscale is rarely reported; fortunately theoretical approaches provide a means to compute interfacial energies on the nanoscale. In the past decade, a number of promising simulation techniques to model nano-interfaces and to compute interfacial energies have been developed. These include phenomenological (analytical) modelling, Monte Carlo, molecular dynamics and quantum mechanical simulations. Here we present an analytical modelling of interfacial energies in nanocrystalline materials1, and a density functional theory simulations of interfacial energies in metal matrix nanocomposite materials2. The size-dependence of interfacial energies of nano-interfaces is well captured by both approaches. At a given temperature, interfacial energies of nano-interfaces increase with the decrease of grain/particle size and change sharply when the grain/particle size is reduced to smaller than a certain critical value. A deep, fundamental understanding of the nanoscale interfacial phenomena would enable tight control of nanostructure morphologies in next-generation materials.

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A Multi-scale, Multi-physics Approach to Modelling of Fusion Welding in Titanium Alloys: *Chinnapat Panwisawas*[1]; Yogesh Sovani[1]; Richard Turner[1]; Jeffery Brooks[1]; Hector Basoalto[1]; [1]University of Birmingham

Microstructural variability induced by the liquid/solid reactions resulting from welding operations are known to influence the mechanical behaviour of a component producing scatter in material properties that can be location specific. The focus of this paper is the development of a microstructure-based approach to the determination of optimised welding parameters. The ICME framework presented is based on an understanding of the causal-and-effect relationships between alloy microstructure, process route and component integrity. The multi-scale, physics-based models developed are applied to fusion welding of Ti-6Al-4V titanium alloy. To identify the weld pool geometry and temperature history, the fluid flow and heat transfer calculation has been first simulated using computational fluid dynamics techniques. A finite element cellular automata model is then used to predict the grain evolution during the weld solidification. Plastic flow is simulated using a microstructure sensitive dislocation-density based crystal plasticity model, which has dependencies on the alpha/beta dispersion. It is demonstrated that model predictions within the welded region are sensitive to the microstructure details and can significant impact upon the overall weld integrity. The predicted flow behaviour is compared with available experimental information.

4:00 PM

Multiscale Modeling using Probabilistic Description of Microstructure: *Veera Sundararaghavan*[1]; John Allison[1]; Anna Trump[1]; Abhishek Kumar[1]; [1]University of Michigan

We present our current progress on the use of reduced order descriptors for modeling microstructure-property relationships in Titanium alloys. We have currently developed methods for sampling and physics-based modeling of three reduced order descriptors with increasing levels of microstructural information: orientation distribution function (ODF), grain size orientation distribution function (GSODF) and the conditional orientation correlation function (COCF). These descriptors are sampled from microstructures from experiments or phase field analysis using monte carlo methods and are subsequently represented using finite element meshes. Equations describing probabilistic constraints (eg. normalization, symmetry) are solved to compute evolution of the underlying probability densities during processing. The approach has been demonstrated for planar (2D) microstructures as well as TiAl alloys by comparing predictions of stress—strain response and texture evolution. A comparison of the simulation speed reveals that reduced order models are significantly faster than full-order crystal plasticity finite element models that use complete microstructural information.

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Phase Field Simulation of Orowan Strengthening by Coherent Precipitate Plates in a Mg-Nd Alloy: Hong Liu[1]; *Jian-Feng Nie*[1]; Yunzhi Wang[2]; [1]Monash University; [2]The Ohio State University

The phase field dislocation model has been used to compute and simulate interactions between basal slip dislocations and coherent β_1 precipitate plates in a Mg-3wt.%Nd alloy that is strengthened exclusively by the β_1 plates. The computed increments of the critical resolved shear stress (ΔCRSS) for samples aged for 10 hours at 523 K agree well with those calculated from the existing strengthening equation for plate-shaped particles. The phase field simulations further indicate that the ΔCRSS value increases with an increase in plate aspect ratio and number density, and that the change of ΔCRSS is not sensitive to the variation of the distribution of β_1 plate diameters when the average diameter of β_1 plates is fixed. When the volume fraction of β_1 plates is constant, the ΔCRSS value for a random spatial distribution of the β_1 plates is approximately 0.78 times of that for a regular spatial distribution.

ICME Models, Tools and Infrastructure I

Monday PM
June 1, 2015

Room: Amphitheater
Location: Cheyenne Mountain Resort

2:00 PM

New Experimental Protocols for Mesoscale Studies of the Transformation of Retained Austenite to Martensite in Dual Phase Steel: *Ali Khosravani*[1]; Surya Kalidindi[1]; [1]Georgia Institute of Technology

Attempts to achieve the goal of higher efficiency in fuel consumption have pushed automotive industries to replace heavy parts with the ones made of lightweight material system or develop the current material to a stronger one. Inasmuch as the large portion of a vehicle is made of steel alloys, a goal of producing a new generation of dual phase (DP) steel with higher strength is desired, leading to weight reduction through thinner part production. However, developing of DP steel requires better understanding of transformation of austenite to martensite during loading. Thus, strain measurements at the microstructural level are essential in studying this transformation. Despite advances in instrumentation and indentation analysis protocols, there are still deficiencies in collecting and interpreting nanoindentation data especially when it pertains to characterizing local response of microscale constituents and interfaces. This work focuses on extracting high value information from indentation measurements through in-situ measurements of orientation changes in the indentation zone. This is accomplished using a special set-up where indentation is performed at the edge of a sample on one face and EBSD measurements are conducted in the highly heterogeneous indentation zone on a perpendicular face. In addition, the plastic strain accumulation with sub-grain resolution is measured with a digital image correlation (DIC) technique on BSE images collecting during indentation. These observations provide critical new quantitative insights into the role of phase boundaries in the mechanical response of DP steels. These new insights will be exploited in the development of new DP steels in future studies.

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Rapid Structure-Property Relationships Using Spherical Microindentation Stress-Strain Curves in Titanium Alloys: *Jordan Weaver*[1]; Surya Kalidindi[1]; [1]Georgia Institute of Technology

Recent advances in nanoindentation data analyses protocols have been able to capture the elastic and plastic anisotropy of single grains and grain boundaries in polycrystalline metals in the form of indentation stress-strain curves. In this study, the same analysis was used to analyze instrumented, spherical microindentation in an effort to establish a high throughput mechanical characterization tool for new materials development. Multiple titanium alloys, both chemical and microstructurally different, were tested using an instrumented indenter with spherical tips of 0.5 and 6.35 mm radii. Both hardness and indentation stress-strain results will be presented in an effort to differentiate between hardness and indentation yield strength. Additionally, indentation structure-property relationships for these select titanium alloys will be compared to compression structure-property relationships to establish grounds for the use of spherical microindentation for high throughput mechanical characterization.

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Microtensile Characterization of Deformation and Failure of Fiber–reinforced Polymer Matrix Composites: *Madhav Kolan*[1]; Jessica Krogstad[1]; Kevin Hemker[1]; [1]Johns Hopkins University

Carbon fiber reinforced polymer matrix composites (PMC) have high stiffness, high strength and low density, which are very useful for automotive, aerospace and other engineering applications. To utilize the full potential of these composite materials their underlying deformation micro-mechanisms and failure needed to be investigated. Predictive models suggests that interfacial bond performance is a key mechanism that governs the transfer of mechanical stresses from the matrix to the composite material; any bond losses leads to deterioration and possible premature failure essentially by intergranular fracture mode. However, the aspects such as fracture initiation and strain localization during mechanical loading are not well understood. In this presentation, we will

show strain maps for crack initiation, propagation and eventual failure under unidirectional tensile loading of PMCs that were extracted from digital image correlation (DIC) during in-situ strain-controlled tensile testing experiments. Further, we will demonstrate the mechanical stresses and localized strains on different stacking sequence of carbon fiber in PMCs for the 0o orientation, 0o/45o and 0o/45o/90o orientations cross-ply. The results presented in this talk have important implications on mechanical stresses and strains associated with different cross-ply of fibers orientation, which can provide for designing and tailoring the PMC materials with improved mechanical properties for a wide range of applications.

3:00 PM

Extending CALPHAD Based Tools with Process-Structure-Property Models to Develop a Computational Materials Design Platform: *Paul Mason*[1]; Q. Chen[2]; A. Engstrom Engstrom[2]; K. Wu[1]; [1]Thermo-Calc Software Inc.; [2]Thermo-Calc Software AB

CALPHAD is a phased based approach to describing the underlying thermodynamics and diffusion in complex, multicomponent systems taking into consideration composition and temperature variation. In the early days of CALPHAD predictions were made based on thermodynamic equilibrium. The approach was then extended to consider diffusion controlled kinetics. More recently, development has focused on predicpitation kinetics and also the modeling of microstructure through phase field. This enables the predictive modeling of process-structure with variation in chemistries essential for materials design. ICME however ultimately needs process-structure-property relationships and new work is now focusing on the integration of process-structure-property models into Thermo-Calc to provide a framework for computational materials design. This presentation will describe the development and integration of such models into Thermo-Calc and new functionality based around a computational materials design platform.

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3D Laboratory-based X-ray Diffraction Contrast Tomography of Polycrystalline Beta Titanium Alloys and Validation to EBSD and Synchrotron: *Erik Lauridsen*[1]; Arno Merkle[2]; Peter Reischig[3]; Christian Holzner[2]; Michael Feser[2]; Kevin Fahey[2]; Henning Friis Poulsen[2]; Leah Lavery[2]; [1]Xnovo Technology ; [2]Carl Zeiss X-ray Microscopy, Inc.; [3]Xnovo Technology

We have demonstrated the ability to derive 3D crystallographic information via diffraction contrast tomography (DCT) within a commercial laboratory X-ray microscope. We will present a method to acquire, reconstruct and analyze grain orientation and related information from polycrystalline samples on a commercial laboratory X-ray microscope (ZEISS Xradia 520 Versa) that utilizes a synchrotron-style detection system for X-ray tomography. Advanced reconstruction and analysis capabilities was enabled through Xnovo Technology GrainMapper3D™ software. To help validate the accuracy of this technique, comparisons with EBSD and Synchrotron DCT, were carried out on polycrystalline Ti-alloys. In doing so independent measure¬ments of grain centroids, grain size, and grain orientations were obtained. Also the angular accuracy of the crystallographic orientations were compared to those obtained using synchrotron DCT and EBSD. We found that the DCT demonstration on laboratory XRM had performance comparable to synchrotron-based approaches. We will present the results of this comparison as well as discuss the boundary conditions of such a method. Here we will also present a selection of laboratory DCT results on Cu, AlSi and Si samples and methods in which this can be correlatively coupled to related techniques for a better understanding of a materials structure evolution at multiple length scales in 4D studies or under in situ environments.

4:00 PM

Integrated Computational Model for Surface Strain Characterization in Stainless Steels and the Experimental Validation: *Lili Zheng*[1]; Wei Wu[2]; Ke An[2]; Wei Yuan[1]; Harsha Badarinarayan[1]; [1]Hitachi America Ltd; [2]Oak Ridge National Lab

An integrated micromechanical based model was developed to characterize the deformation phenomenon for stainless steels under various loading conditions. To acquire the prerequisite single crystal stiffness, in situ neutron diffraction measurement was conducted and the lattice strain history was obtained as a function of applied stress. The modeling framework begins with the modified Kronor's model to calculate the single crystal stiffness by least square fitting to the measured orientation-dependent elastic constants from the neutron data. Additionally electron backscatter diffraction (EBSD) was performed to identify the material microstructure on sample surface before deformation. A crystal plasticity finite element method (CPFEM)-based micromechanical model was developed to predict the deformation behavior of material on sample surface under various loading conditions. The crystal stiffness obtained from the previous modified Kronor's model, and the material grain structure and orientation from the EBSD measurement were embedded into the CPFEM model. . On the other hand, atomic force microscopy (AFM)-based experimental approach was developed to determine the surface strain from the measured surface topography. The results from the integrated modeling methods and the AFM-based experimental approaches are compared in this study.

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Investigating the Role of Microstructure in HCF and VHCF Regimes Using Ultrasonic Fatigue Methods: *J. Wayne Jones*[1]; Jason Geathers[1]; Christopher Torbet[2]; Tresa M. Pollock[2]; Samantha Daly[1]; [1]University of Michigan; [2]University of California Santa Barbara

Modeling fatigue crack initiation and early crack growth to accurately predict fatigue lifetimes remains a significant challenge, especially in the high cycle or very high cycle regime, This is especially true when crack nucleation and small crack growth at the scale of the microstructure features occupy most of fatigue lifetime. We review the use of ultrasonic fatigue methods to both accelerate investigations of these phenomena and to probe the microstructure level mechanisms of crack initiation and small crack growth and to identify critical microstructure features or neighborhoods that control fatigue behavior. Examples of the influence of microstructure variability on fatigue behavior in the high cycle and very high cycle regimes will be drawn from recent work on the role of microtexture in near-alpha titanium alloys and investigation of the role of microstructure neighborhoods on crack initiation and early growth in Rene 88. Finally, we describe the development and use of a new ultrasonic fatigue instrument that operates in a scanning electron microscope to provide the capability for rapid high-resolution observation of crack initiation and early crack propagation phenomena. The use of this experimental arrangement in an environmental SEM to investigate the influence of environment on crack initiation and propagation in Ti-6242S will be described in detail.

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Resonance Behavior Changes with Damage in Nickel-Based Superalloys: *Brent Goodlet*[1]; Tresa Pollock[1]; [1]University of California, Santa Barbara

Numerous ultrasonic nondestructive evaluation (NDE) techniques exist to probe structural components, all with varying levels of accuracy and inherent limitations. Herein, ultrasonic resonance, commonly referred to as resonant ultrasound spectroscopy (RUS), is investigated as a NDE technique for nickel-based superalloys. Changes in component microstructure, material properties, geometry, stress state, temperature, and orientation all affect resonance behavior. While the fundamentals discussed apply broadly to most structural materials, finite element (FE) models in this study are used for simulating damage relevant to multi-phase multi-component nickel-based superalloys exposed to high temperatures. Once the isolated damage mode is simulated through FE models, the resulting change in resonance behavior can be deduced through comparison to an undamaged model. A focus on how FE models enable the identification of distinct resonance modes with deflection characteristics that are more sensitive for NDE will be discussed. Model development and material property definitions are addressed, as are length scales relevant to ultrasonic resonance for NDE. Dominant mechanisms affecting resonance are proposed and studied first through modeling. Then model predicted shifts in resonance frequencies are validated with controlled experiments on superalloy samples before and after high temperature exposure. Measure to model comparisons work to inform our understanding of measurement sensitivities, rule out inconsequential mechanisms not responsible for resonance behavior evolution, and inform future model development in hopes of better understanding the NDE potential of RUS.

Poster Session I

Monday PM
June 1, 2015

Room: Colorado I
Location: Cheyenne Mountain Resort

PI-1: An Integrated Finite Element Framework for the Hole Piercing to Hole Expansion Process of AA6111-T4 Sheets: *Xiaohua Hu*[1]; Xin Sun[1]; Sergey Golovashchenko[2]; [1]Pacific Northwest National Laboratory; [2]Ford Motor Company

Similar to the studies of tensile stretchability of previously trimmed sheet by Hu et al., an integrated finite element framework is used to study the process from hole piercing to hole expansion tests with the aim of studying the influences of the cutting affected zone near the hole edge out of the hole piercing on the hole expansion ratio (HER) of later hole expansion tests. With the use of damage model and parameters calibrated from the previous tensile stretchability studies, the calculated HER correlates well with experimental measurement in variation with hole piercing clearances. The hole piercing model show that there are no or very small burr for clearances less than 20%, which corresponds well with the facts that measured and FE calculated HER is not very sensitive to piercing clearance which it is smaller than this value. The HER values of clearances of 30% and 40% are considerably smaller.

PI-2: Atomistic Modeling of Epoxy CNT Nanocomposites: Veera Sundararaghavan[1]; *Nicholas Fasanella*[1]; [1]University of Michigan

Molecular dynamics simulations are performed to compute properties of cured epoxy resins reinforced with carbon nanotubes. The current tools available allow building of energy equilibrated epoxies with cross linking conversion similar to those seen in structural epoxies. These structures can be tested virtually for the purposes of materials selection and design even before synthesis of the polymer. We have previously predicted several properties of resins, including coefficient of thermal expansion, thermal conductivity, elastic modulus and yield strength through molecular dynamics simulations and compared to experiments. Results from molecular dynamics simulations performed on nanotube reinforced cross-linked epoxy matrix will be shown. Simulations are carried out using CVFF force field in LAMMPS. Nanocomposites were made by adding functionalized and non-functionalized carbon nanotubes to the epoxy matrix. Through MD simulations, we develop means to build simulation cells, perform annealing to reach correct densities, compute thermomechanical properties and compare with experiments.

PI-3: CALPHAD-based and Experimental Investigations of Microstructures in Austenitic Heat-resistant Cast Steels for Exhaust Component Applications: Yinhui Zhang[1]; Mei Li[2]; Larry Godlewski[2]; Jacob Zindel[2]; *Qiang Feng*[1]; [1]University of Science and Technology Beijing; [2]Ford motor company

To comply with stricter environmental and fuel consumption regulations, exhaust components for gasoline engines of automobiles are required to withstand exhaust gas temperatures as high as 1050 °C. Thus, it is competitive to develop new cast steels with higher heat-resistance and durability than conventional materials. Precipitation strengthening is one of the primary strengthening methods for new alloy designs, where Nb(C,N) carbonitrides are generally introduced due to their extremely high thermal stability. In this study, the carbon and nitrogen effect on microstructures in four Nb-bearing austenitic heat-resistant cast steels was examined through complementary CALPHAD-based and dedicated experimental investigations. Thermodynamic calculations were performed using JMatPro software to predict the fraction of equilibrium phases in the alloys as well as the compositions of phases at relevant temperatures. The solidification sequence of alloys was predicted via the Scheil-Gulliver module attached to the software. It revealed that the addition of nitrogen increased the precipitation temperature of Nb(C,N) carbonitrides, even higher than the liquidus temperature, and consequently affected the morphology, distribution and size of the precipitates. Meanwhile, the content of carbon and nitrogen had a strong influence on the formation of delta-ferrites, which would go through a significant amount of solid transformation from growth of gamma-austenites. The compositional effect on solidification and precipitation behaviors as well as strengthening mechanisms during creep testing at 1000 °C and 50 MPa will be discussed. The information about compositional and microstructural effects on creep properties in austenitic heat-resistant cast steels is helpful to modify alloys with better microstructures.

PI-4: Coating on Performance: *Dieter Heumannskaemper*[1]; [1]Morgan Advanced Materials

Morgan Advanced Materials has developed several coatings for different applications. By manipulating the particle size density and the chemical composition of the different coatings, the bonding strength and types between the coating and the crucible surface is optimised and adapted to the different applications.These coatings with varied compositions have varying functions ranging from: Dross adhesion reduction (in aluminium application); reduced impurity leaks into the melted metal from crucible body(aluminium and Al-Alloys, precious metal);increased erosion resistance of the crucible (copper and copper alloys and when fluxes are used).

PI-5: Degradation of Crucible Properties and Impact on Energy Consumption During Operation: Dieter Heumannskaemper[1]; *Mirco Pavoni*[1]; [1]Morgan Advanced Materials

Development of an isostatically pressed graphite crucible with a high thermal conductivity. Due to the well developed mixing and pressing procedures, the crucible has a homogeneous structure throughout. The high thermal conductivity leads to a shorter melting time and reduced energy consumption per amount of melted metal. Additionally a well developed glaze for oxidation protection increases the lifetime of the crucible. Several Case studies will be presented.

PI-6: Design of Co-free Cemented Carbides: *Martin Walbrühl*[1]; John Ågren[1]; Annika Borgenstam[1]; [1]KTH - Royal Institute of Technology

The replacement of Co as binder phase material in cemented carbide systems is motivated by several reasons. Beside the possible reduction of material costs and enhanced materials properties the main driving force for the replacement is due to potential restrictions in the European regulations regarding Co. Since Co has been identified to possibly be harmful to health and may be restricted in Europe, the cemented carbide industry needs to focus on the development of alternative binder systems to replace Co. Beginning of the 1980's first systematical investigations of alternative systems based on Fe and Ni, as alternative binder materials, have been carried out. Anyhow without a strong driving force to replace Co, as it is occurring now, a generally sufficient material for the replacement has not been found yet. Within the latest published research different alternatives have been shown which could lead to promising solutions for the cemented carbide industry. The important sector of metal cutting still suffers from a lack of suitable binder phase replacement. The present work, based on the study of earlier research, identifies the crucial points for the materials developing focusing on metal cutting applications. A computational material design approach has been applied by using thermodynamic and kinetic models involving DFT, DICTRA and Calphad-type of calculations. The new binder phases have been designed with the focus on tailor made material properties which are desired for metal cutting applications. Promising material candidates have been examined experimentally.

PI-7: Effect of Die Design Parameters on the Stresses Generated during the Closed Die Forging Process: *Santosh Kumar*[1]; Atul Patil[1]; Shreyas Kirwai[1]; [1]Bharat Forge Limited

In closed die forging, die cost amounts approximately 10-15% of the total forging cost. Die cracks, owing to the high tensile stresses generated during forging, has a major influence on the die life. The die life can be enhanced by selection of an appropriate die material and proper die design. Appropriate die design leads to reduction of detrimental tensile stresses at the critical locations by reducing stress concentrations. Now a days, metal forming simulation based on the Finite Element Method has replaced the costly, tedious, time consuming shop floor trials. In the present work, effect of different die design parameters such as Root Radius (RR) of the die cavity, Parting Line Radius (PLR), Die Width (DW), Die Height (DH) and % Yield (% Y) on the developed tensile stresses is studied in the commercial forging simulation software FORGE. Simulation results show that modification in RR and DW has a major effect on the developed tensile stresses but modification in PLR and DH has a minor effect on the same. Tensile stress increases with increase in %Y up to a certain value beyond which the same significantly decreases.

PI-8: Effect of Shape Oscillations on the Stability of a Particle Laden Bubble during Rising: *Prithvi Yesudas*[1]; Sabita Sarkar[1]; [1]Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai - 600036

Stability of a particle laden bubble and its stable rise plays a major role in particle recovery to slag phase during steel making operations. To understand the effect of shape oscillations on the stability of the particle laden bubble, a mathematical model is developed based on Eulerian-Lagrangian approach. In this model particles are treated as discrete phase and VOF method is used to describe the evolution of bubble in the liquid phase. Predicted shape oscillation of the particle laden bubble is compared with experiments where shape oscillations of the particle laden bubble during rising is captured using high speed camera. The Weber number for a stable bubble particle aggregate and the corresponding frequency of fluctuations is determined and the influence of parameters like particle size , bubble size and bubble rise velocity on forming a stable bubble-particle aggregate is studied.

PI-9: Efficient Degassing for Aluminium Melting: Dieter Heumannskaemper[1]; Mirco Pavoni[1]; *Arjoon Vohra*[1]; [1]Morgan Advanced Materials

The efficient removal of dissolved hydrogen and impurities from the aluminium melt is of a major concern in the casting industry. The newly developed isostatically pressed, single-bodied, carbon-bonded silicon carbide rotor showed a significant improvement in the oxidation resistance and lifetime over existing products. The special rotor head design also improves the formation and homogeneous dispersion of gas bubbles leading to improvements in degassing rates, degassing consistency across the lifetime of the rotor and a narrower melt density range after degassing.The increased lifetime and degassing performance are benefits that effectively reduces the cost of ownership of the new degassing rotor. Several case studies will be presented.

PI-10: Experimental and Numerical Determination of the Fracture Energy of Carbon Fiber Reinforced Phenolic Resin-based Plastics Composites: *Khurram Iqbal*[1]; [1]Dalian University of Technology

In this paper, we have verified the validity of some formulations allowing the determination of the fracture energy of carbon fiber reinforced phenolic resin-based plastics (CFRP) composites. The GIIC is chosen as fracture characterizing parameter which is experimentally determined by considering a multiplying form that is numerically evaluated using a finite element method. The numerical results are compared to the experimental data, and a good agreement has been observed. The specimen geometry was used to determine the mode II delamination fracture energy.

PI-11: Experimental Verification for Solid Fraction Measurement in Semi-solid Silver Metal Processing in Comparisons with Theoretical Thermodynamics Modeling: *Pun Wirot*[1]; Boonrat Lohwongwattana[1]; Ekasit Nisaratanaporn[1]; [1]Chulalongkorn University

The actual volume fraction of the solid in semi-solid metal processing is critical to achieving the most effective semi-solid metal processing. The semi-solid slurry with different solid fractions shows different ability to fill molds. To determine suitable processing conditions for semi-solid sterling silver (92.5 wt.%), thermal analysis (TA), experimental verification in actual investment casting machine as well as thermodynamics models were performed. Classical Gibbs free energy calculation and Scheil-Gulliver modeling were used to estimate the relationship between solid fraction and temperature. In order to obtain the relationship between temperature and solid fraction, comparisons were made amongst different techniques. The investigated 925 silver alloy was heated to 950 degree Celcius, and gas bubbling apparatus was used to introduce Ar gas into the melt. Cooling curves for the metal were recorded with two thermocouples, one at the center of the melt volume and one beside the containing crucible wall. Different cooling curves and temperature profiles are presented from various tests to compare solid fractions. It was found that the latent heat of fusion strongly affected the solid fraction in addition to thermodynamic contribution. To adequately express the solid fraction relationship, the thermodynamics modeling needed modifications that took into account the cooling effects as well as temperature gradient in the crucible. Keyword: Semi-solid processing, sterling silver, thermal analysis, thermodynamic models

PI-12: Exploring the Performance-Property-Structure Solution Space in Friction Stir Welding: *Chung Hyun Goh*[1]; Adam Dachowicz[1]; Janet Allen[1]; Farrokh Mistree[1]; [1]University of Oklahoma

Many attempts have been made to fabricate dissimilar materials using materials joining processes. Welding is a thermo-mechanical joining process which involves microstructure fabrication through a melting process. The welding process is widely used in industrial fabrication applications. This process also plays an important role in joining multi-layers in additive manufacturing. By way of example, we plan to use friction stir welding (FSW) since it can effectively avoid material defects such as voids arising from the solidification process, compared to liquid-state welding. Several factors influence weldability in the FSW process. These include processing conditions and processing parameters like melting temperature, axial force, and tool rotational speed. The temperature history effect significantly affects residual stresses and distortion problems during the FSW process. Therefore, we focus on improving the strength and hardenability by considering the temperature history effect in the FSW process. We use the set-based inverse design (SBID) developed by us to explore the structure/property/performance solution space. In this paper, we describe the salient features of the SBID method and illustrate its efficacy in the context of Integrated Computational Materials Engineering domain.

PI-13: Force Modelling for Temperature Field determination During High Speed End-Milling of Superalloys: *Sunday Ojolo*[1]; Oluwole Adesina[2]; Gbeminiyi Sobamowo[1]; [1]University of Lagos; [2]Yaba Colege of Technology

Temperature field in metal cutting process is one of the most important phenomena in machining process. Temperature rise in machining determines other cutting parameters such as tool life, wear, thermal deformation, surface quality and mechanics of chip formation. It is therefore very important to investigate the temperature distribution on the cutting tool–work piece interface in end milling operation. Most studies previously carried out on the temperature distribution model analysis were based on analytical model and with the used of conventional machining which is continuous cutting in nature. The limitations discovered in the models and validated experiments include the oversimplified assumptions which affect the accuracy of the models. In metal cutting process, thermo-mechanical coupling is required and to carry out any temperature field determination successfully, there is need to address the issue of various forces acting during cutting and the effect on the tool- work piece interface. Most previous studies on the temperature field either neglected the effect of friction or assumed it to be constant. The friction model at the tool-work interface and tool chip interface in metal cutting plays a vital role in influencing the modelling process and the accuracy of predicted cutting forces, stress, and temperature distribution. In this work, mechanistic model was adopted to establish the cutting forces and also a new coefficient of friction was also established. This can be used to simulate the cutting process in order to enhance the machining quality in the area of surface finish and monitoring the wear of tool.

PI-14: High Entropy Nickel Superalloys Designed via the CALPHAD Method: *Joseph Licavoli*[1]; Paul Jablonski[1]; Jeff Hawk[1]; [1]Department of Energy

Nickel superalloys represent a class of advanced high temperature materials which have undergone several improvements in recent decades. Most recent efforts to modify nickel super alloy performance focus on introduction of new secondary phases or modifications to phase fractions. High entropy alloys are a new class of multicomponent materials in which configurational entropy limits the number of equilibrium phases and thus results in enhanced stability. These alloys have displayed several appealing qualities including high temperature strength and creep resistance. The current study makes use of the CALPHAD technique to design several new nickel superalloys with phase fractions similar to conventional wrought alloys, but with an FCC matrix whose configurational entropy was comparable to high entropy systems. Large scale (7kg) ingots were cast using vacuum induction melting techniques with care taken to minimize tramp elements including sulfur. Ingots were then given computationally based homogenization heat treatments in order to achieve local chemistry within 1% of nominal. Following this they were hot-worked into slabs in order to produce a fully wrought structure. Tensile tests were then carried out at several temperatures ranging from room temperature to 1073 K. Metallographic results from processing trials were compared to CALPHAD estimates and the current limitations of this approach for high entropy alloy design will be discussed. Mechanical test results were also compared to those of several commercial wrought super alloys.

PI-15: Hot Deformation Behavior and 3D Processing Maps of Extruded AZ61 Magnesium Alloy: *Juqiang Li*[1]; [1]Shanghai Jiao Tong University

The hot deformation behavior of extruded AZ61 magnesium alloy was investigated using the hot compression tests in the temperature range of 250–400 °C and strain rate of 0.001–1 s^{-1}. The apparent activation energy of deformation was calculated to be 144.85 kJ/mol and a constitutive equation that describe the flow stress as a function of the strain rate and deformation temperature was developed. Dynamic materials model (DMM) was employed to construct the 3D power dissipation maps with a view to finding optimum hot working parameters and evaluating the mechanisms of hot deformation, and Prasad's instability criterion, Gegel's stability criteria were used to build the 3D instability maps. It was found that the power dissipation map exhibits two deterministic domains representing dynamic recrystallization (DRX). Both these are in the strain rate range 0.003–0.1 s^{-1}, with one in the lower temperature range (250–300 °C) and the other in the higher temperature range (350–400 °C). Detailed comparison of the instability maps coupled with microstructural observations revealed that the instability map developed as per Prasad's instability criterion was quite different from that developed according to Gegel's stability criteria and the former was found to provide more reliable prediction of unstable regions than the latter.

PI-16: Performance Enhancement of SiC Heating Elements by Virtue of Simulation: *Yongwoo Kwon*[1]; Youngjae Cho[1]; Jonghuck Lee[1]; Seung-Yong Lee[2]; Young-Min Kong[3]; [1]Hongik University; [2]Korea Institute of Science and Technology; [3]University of Ulsan

The SiC heating element achieves great reliability and power efficiency in dehydrating or water boiling systems unlike the conventional Ni-Cr that cannot make a direct contact with water or vapor due to its poor corrosion resistance. Our SiC heating elements are fabricated by extrusion process. Raw materials including SiC powders, additives, and solvent are mixed to prepare paste which in turn goes through a mold with pressure. Finally, we get a pipe that has a certain cross-sectional shape depending upon the mold shape. In our case, it is a long cylinder with many regularly spaced rectangular holes, like a mesh, through which fluid can pass. Typically, it has about one hundred holes per square inch. This cylinder is cut into pieces. All the pieces are dried and sintered. The microstructure is porous such that it can be regarded as a composite with SiC phases and pores. The microstructure greatly influences electrical and thermal conductivities. In this talk, we will present on the systematic study to find the microstructure-performance relationship for the SiC heating element. An FEA software whose inputs are the geometry of the heating element and the properties of the SiC-pore composite was used to analyze the heat generation and transfer. Our own codes were used to calculate the effective conductivities from those of a SiC phase and a pore, and to model the evolution of the microstructure during sintering. In this way, we could estimate the performance of the heater as a function of microstructure.

PI-17: Phase-field Modeling of Morphological Evolution of a Charged Particle: *Dong-Uk Kim*[1]; Hee-Chul Yang[1]; Pil-Ryung Cha[1]; [1]Kookmin University

Electrostatic force is one of the strongest long-range interactions in the nature. Sometimes it induces extremely complex pattern formation including fractal-like growth and corrosions. But, there are few researches sufficiently explaining the phenomena because of its theoretical complexity. Even, in electrostatic theory, there is no general theory to calculate surface charge density distribution of an arbitrary shaped charged conductor in equilibrium both analytical and numerical ways. This lack of knowledge in electrostatics makes hard to develop theoretical or numerical models describing practical simulation tools on electrostatic or electrochemical systems. In this study, based on electrostatic energetics, pattern formation of a conducting and non-conducting charged particle was simulated by phase-field approach with mass conservation and charge conservation condition. Especially for a conducting charged particle, surface charge density distribution of arbitrary shaped interface was calculated.

PI-18: Prediction of Particle Recovery and Wall Stress due to Submerged Swirling Gas Jet-liquid Interaction: *Vishnu Mantripragada*[1]; Sabita Sarkar[1]; [1]Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai - 600036

Gas jet is often injected in liquid metal pool to recover the particles to the slag phase in steel making process such as oxygen steel making, ladle refining and tundish flotation. The current work involves study of hydrodynamics and its effect on particle recovery to the slag phase due to interaction of submerged gas jet with liquid pool. A submerged swirling gas jet is considered in this study. The gas and liquid phases are simulated by Eulerian approach using VOF model and the particle or impurity phase is simulated using Lagrangian approach. The effect of swirling flow on the time taken for particle recovery to the slag phase is investigated for various positions of the lance. The stress generated on the ladle walls due to the turbulence induced by the gas jet in the liquid pool is also quantified.

PI-19: Structure-Property Modeling Tools for Triplex Mo-Si-B Alloys: *Kyle Brindley*[1]; Richard Neu[1]; [1]Georgia Institute of Technology

Refractory metals and their alloys offer higher temperature alternatives to Ni-base superalloys. In particular, Mo-Si and Mo-Si-B intermetallics offer excellent oxidation and creep resistance at temperatures up to 1400\176C. However, these intermetallics present a significant design challenge due to their low ductility and low fracture toughness at room temperature. A balance of high temperature and low temperature mechanical properties may be achieved in Mo-Si-B alloys by including the \945-Mo phase in addition to the intermetallic phases. Balancing the mechanical properties requires proper microstructure optimization. Through the use of finite element simulations, microstructure-sensitive structure-property modeling allows for this optimization to be done faster and less expensively than traditional methods. Three modeling tools are required for microstructural modeling: microstructure generators to re-create statistically realistic microstructures, crystal viscoplasticity constitutive equations implemented for use with finite element solvers, and post-processing tools to evaluate important mechanical properties and fatigue at a variety of microstructural features. A preliminary investigation into the development and application of these tools for triplex Mo-Si-B alloys is reviewed here by first developing these tools for the \945-Mo phase and calibrating the constitutive equations for the \945-Mo phase as a function of Si content, temperature, and strain rate. Following the calibration of the \945-Mo phase constitutive equations, an initial model for the fully triplex microstructure may be achieved by treating the intermetallic phases as purely elastic. Such an assumption can be supported by the very small amounts of plastic deformation observed in the intermetallic phases of triplex Mo-Si-B alloys.

PI-20: Synthesis and Characterisation of Al Doped ZnO Nanoparticles: *Chitrashi Mahajan*[1]; [1]NIT

Al doped ZnO nanoparticles have been synthesized by co-precipitation method at temperature of 500oC for 2 hours in air. The synthesized samples were characterized by powder X-ray diffraction (XRD), FE-SEM/EDS,

and UV–Visible spectrophotometer. The prepared nanoparticles exhibit a hexagonal wurtzite structure with an average particle size of 26 nm as evident from XRD measurements. The calculated average crystalline size of particle varied from 20 to 39 nm with increase in Al concentrations. The increase in lattice parameters reveals the easy fit of Al into ZnO lattice. It was observed that the Al doped ZnO nanopowder particles exhibit higher transmittance i.e. above 77 % at 400 nm wavelength as compared to the un-doped ZnO nano powder particles (70 %) due to its smaller crystal size (23.9 nm) as compared to un-doped ZnO powder particles (77.4 nm). It is due to quantum confinement effect leading to the variation in density of states (DOS) with nanosized particles Key words: Al doped ZnO nanoparticles; XRD; FE-SEM/EDS; Spectrophotometer

PI-21: The Finite Element Analysis to Improving the Effect of Thick Slab Continuous Casting Bulging: *Weihua Wang*[1]; [1]Shougang Research Institute of Technology

The different degree of slab narrow face bulging phenomenon (maximum bulge size of 10 ~ 20mm) has been appeared in the production of 300mm ~ 400mm thick section of continuous casting slab of a factory. The commercial software ANSYS has been used according to the above by author to analysis two schemes about adding the foot roller in the lower of slab narrow surface foot roller or adding the nozzle. The results shows that: The slab bulging deformation can be effectively improved by the two schemes: 1) The maximum bulge size slab were 5.93mm and 2.53mm by adding 2 or 3 couple foot roller; 2) The slab shell thickness has been increased after adding the nozzle. When the slab shell thickness at the end of the straight section are 160mm, 180mm and 200mm, the maximum bulge size of slab are respectively 4.56mm, 3.56mm and 2.92mm.

PI-22: Towards Plug & Play in ICME – Pathways Towards Communication Standards and Interface Specifications: *Georg Schmitz*[1]; [1]Access e.V.

Integrated Computational Materials Engineering - ICME - by its nature draws on the combination and the simultaneous or consecutive use of a variety of software tools. In spite of ICME currently emerging as a new and powerful discipline, coupling of different software tools is still in its infancy and represents an issue consuming significant effort in terms of time and workforce if a coupling is realized at all. The presentation will introduce ICMEg – the Integrated Computational Materials Engineering expert group. This coordination activity of the European Commission aims at developing a global open standard for information exchange between the heterogeneous varieties of numerous – academic and commercial - simulation tools. Following a short discussion on the benefits of such a global and open standard for the different communities, the presentation will detail the approach being taken by ICMEg towards its realization. Starting from building up a scientific network of stakeholders interested in boosting ICME into industrial applications, the major scope of ICMEg is to generate a global and open standard for information exchange in ICME settings. As the expertise of a single institution – however – cannot cover all aspects to be considered when elaborating suitable standard formulations for the heterogeneous variety of models and tools, a collective and global effort of different communities is mandatory. This collective effort has been initiated and will be further moderated by the ICMEg consortium. For this purpose a forum has been established on the ICMEg website.

Applications III: Composites and Non-Ferrous

Tuesday AM
June 2, 2015

Room: Colorado II
Location: Cheyenne Mountain Resort

8:00 AM

Exploiting Interfaces in Multi-scale Topology Optimization for ICME: *Natasha Vermaak*[1]; [1]Lehigh University

Recent advances in the mathematical formulations for structural design optimization using the level set methodology have enhanced the treatment of a key feature introduced and typically ignored in multi-material optimization models: solid interfaces. Material interfaces play a pivotal role in the actualperformance of a composite multi-material structure, often dictating lifetime and failure characteristics, tolerances and processing choices. Topology optimization offers a methodology for arranging multiple materials in space to meet loading and design requirements. This study directly incorporates models that relate how manufacturing or processing affect interface properties into the structural optimization. The motivation is to highlight the influence of manufacturing and processing-dependent interface effects on optimal design at multiple scales. Several elastic and thermoelastic engineering problems ranging from structural components for Big Area Additive Manufacturing (BAAM) to the design of cellular microstructures are used to demonstrate significant performance changes that are linked to local interface properties.

8:20 AM

Integrated Computational Methods for Composites Materials (ICM2): Lessons Learned From Integration Planning and Feasibility Demonstrations: *Lara Liou*[1]; [1]GE Aviation

General Electric Aviation and Lockheed Martin Aeronautics have teamed through an Air Force Research Lab program to conduct a demonstration of an Integrated Computational Materials Engineering digital framework that links material processing, property, and structural relationships to account for processibility, manufacturability, and system performance with the goal of demonstrating that the usage of integrated models can contribute to future airframe and engine designs with dramatic reductions in development time and cost. Both engine and airframe Foundational Engineering Problems will be demonstrated through a common digital framework to be developed and validated on increasingly complex articles. The modeling tools which cover composite process models, localized mechanical behavior models, and global design models (Convergent Manufacturing Technology's COMPRO CCA, Autodesk's Autodesk Simulation Composite Analysis, and an Abaqus based University of Michigan micromechanics model) are centrally linked via a commercially available model integration interface (Phoenix Integration's ModelCenter). Detailed plans of what data will be passed among the various models as well as how it will be passed have been completed. Creation of these detailed process maps and simple feasibility demonstrations have raised inherent technical and logistical challenges to integrating commercially available, multi-scale models. Robust model integration methods to address these challenges will be discussed.

8:40 AM

Use of a Computational Method to Develop a New Composite Matrix Chemistry with Improved Performance: *Stephen Christensen*[1]; [1]Boeing Research & Technology

Using computational methods and experiments and the teachings of a continuum level concept known as Onset Theory, we have established a methodology for the prediction of composite performance that allows materials development by design. The method is demonstrated with a matrix formulation development that validates the relations we have established between composite performance and constituent properties. The use of molecular dynamics for thermoset matrix formulation required the development of several new techniques. Our results show that composite performance is predictable and improvements are achievable through the proper selection of resin components.Reference: Computational formulation of a new composite matrix; S. Christensen, R. D'Oyen, Scripta Materialia vol 70 (2014) pp 18-24

9:00 AM

Manufacturing Process Induced Effects in Mechanical Behavior of Carbon FRPCs: *Marianna Maiaru*[1]; Royan D'Mello[1]; Pavana Prabhakar[2]; Folusho Oyerokun[3]; Matthew Hockemeyer[4]; Li Zheng[4]; Anthony Waas[1]; [1]University of Michigan, Ann Arbor; [2]University of Texas, El Paso; [3]GE Aviation; [4]GE Global Research

The manufacture of carbon fiber reinforced polymer composites (FRPCs) involves curing of the matrix. The mold with the fibers and liquid resin undergoes a prescribed temperature cycle; during this process, as the matrix hardens, it shrinks due to the formation of polymer networks and crosslinks. Also, since the reaction is exothermic, thermal stresses develop. Depending on the severity of cure shrinkage and thermal stresses, the material can degrade during the process. To simulate the curing, a physics based model is incorporated into the finite element method. For this purpose, representative unit cells containing 2 to 20 carbon fibers are chosen in hexagonally packed and random packed configurations. Using these models, the degree of damage in the matrix is computed for various cure cycles; the fiber volume fraction and randomness associated with fiber packing are taken into account. At the end of each curing cycle, the strengths of the RUCs are determined by subjecting the cured model to various "virtual" loading programs, such as transverse tension, transverse compression, uniaxial tension and so on. Damage leading to fracture during curing and also during the subsequent mechanical loading is introduced using the Bazant-Oh crack band model. The effect of fiber volume fraction and fiber packing on the strengths are studied. Insights into some important variables that affect degree of damage during cure as well as uncertainty in strength values of the cured RUC are provided.

9:20 AM

Capturing Size Effects in Composites Using Progressive Failure Stochastic Simulation: *Seyed Hamid Reza Sanei*[1]; Ray Fertig[1]; [1]University of Wyoming

In the design of composite structures, the results from testing small coupons are used in design of actual structures. According to the homogeneity assumption, the volume average strength is not dependent on specimen size and the results are applicable to other sizes. However, experimental findings have shown that the strength is sample size dependent, such that larger samples have lower strength. This phenomenon is the so-called size effect. The common approach to address the problem is to scale the predicted strength based on the results of small coupons. The two available analytical scaling methods are Weibull statistical strength theory and the fracture mechanics approach. One of their intrinsic shortcomings is that they are only applicable for tensile loading and yield poor predictions in compression and shear loadings. This study proposes a methodology for capturing size effects in strength by employing progressive failure Monte Carlo finite element simulation. First, each element is assigned a fiber volume fraction from the actual distribution determined from segmentation of SEM images. Then the intrinsic strength of a fixed element size is determined. Finally, the effect of changing sample size will be investigated to determine the appropriate scaling behavior, a priori, for predicting failure of larger samples under complex load states. The normal and shear strengths in all direction for two different sized unidirectional carbon epoxy composites will be predicted and compared with experimentally measured results for validation.

9:40 AM Break

10:00 AM

Application of Multi-Scale Fatigue Models in Lightweight Metal Castings: *Qigui Wang*[1]; [1]General Motors

Lightweight castings are increasingly used in critical structural applications which are often subjected to cyclic loading during service. Fatigue property of the lightweight castings has become a critical design criterion. Fatigue performance of lightweight castings strongly depends upon the presence of casting flaws and characteristics of microstructural constituents. The existence of casting flaws significantly reduces fatigue crack initiation life. In the absence of casting flaws, however, crack initiation occurs at the fatigue-sensitive multi-scale microstructural constituents. This paper discusses the multi-scale fatigue (MSF) models developed and their application in lightweight aluminum and magnesium castings.

10:20 AM

Modelling Stress-assisted Grain Oxidation Ahead of a Crack in a Nickel-based Superalloy: *Chizhou Fang*[1]; Hector Basoalto[1]; Hangyue Li[1]; Steve Williams[2]; Hugh Evans[1]; [1]University of Birmingham; [2]Rolls-Royce plc

Oxide formation along grain boundaries ahead of the crack tip and its rupture is a mechanism proposed for environmentally assisted time dependent crack growth at high temperatures in nickel-based superalloys for rotor disc applications. A fully coupled mechanical-diffusional finite element formulation is proposed in the current study for stress-assisted grain boundary oxidation ahead of a crack tip. Oxide formation is modelled through a multi-component diffusion formulation, where appropriate source/sink terms have been added to the continuity relations describing the concentration fields. The influence of plasticity and creep on the oxide growth kinetics and stress fields in the vicinity of the crack tip are also investigated. The predicted oxide morphologies ahead of the crack tip are shown to be in good agreement with previous experimental results.

10:40 AM

Polymers on the Edge of Metallic Conductivity and Their Aerospace Applications: *Ekaterina Badaeva*[1]; Patrick Kinlen[1]; Ofer Alves[1]; [1]Boeing

Inherently conductive polymers (ICPs) have been the subject of a great deal of research since their discovery and initial development about three decades ago. ICP-based materials have been found to have high potential for a variety of aerospace applications including electrostatically dissipative coatings for canopies and surfaces, radar signature, next generation wiring, conductive composites, appliques, lightning protection and high power energy storage systems. It is understood that the proper combination of chemical composition of the polymer along with processing to ordered and oriented structures can produce materials with especially high conductivity and stability which are on the edge of truly metallic behavior. Conducting polymer compositions based on polyanilines and poly(3,4-alkylenedioxythiophenes) were recently demonstrated to have electrical conductivities reaching into the hundreds of S/cm. We combine multi-scale modeling techniques with high-quality synthesis and analytical methods to develop a deep understanding of structure-property relationships in this class of ICPs with the ultimate goal to enhance existing conductivities to thousands of S/cm and provide processable and stable conducting coatings. Our efforts involve the optimization of material composition, polymerization method, doping procedure and processing techniques of polyaniline. Since structural defects can scatter charge carriers as they move through a material and reduce conductivity, our work is directed towards solution processable polymers with strong pi-stacking, high molecular weights, and purity in both repeat-unit structure and end-group identity. Specific formulation requirements based on the potential applications will also be discussed.

11:00 AM

Yield Strength Model for Undercooled Aluminium Alloys Based on Calorimetric In-situ Quenching Experiments: *Michael Reich*[1]; Philipp Schumacher[1]; Benjamin Milkereit[1]; Olaf Kessler[1]; [1]University of Rostock

Undercooled supersaturated aluminium alloy 6082 has recently been investigated during in-situ quenching experiments by means of differential scanning calorimetry and thermomechanical analysis. Calorimetry resulted in a continuous time-temperature-precipitation diagram [1] and thermomechanical analysis in stress/strain curves, which have successfully been implemented in a quenching simulation [2]. In this work, the above results have been correlated. Supersaturation of the undercooled aluminium alloy 6082 has been determined from calorimetric data. Next a solid solution strengthening model has been used, to calculate yield strength from supersaturation. The model has further been extended by a temperature dependent term. Yield strength has been computed for a broad range of quenching rates and quenching end temperatures. Results have been compared with experimental data from quenching & deformation dilatometry and found to correlate very well. This yield strength model and the calorimetric calibration method can be transferred to other alloys. It can significantly improve quenching simulation including residual stresses and distortion. These simulations require mechanical properties of undercooled supersaturated aluminium alloys, which can´t be measured by conventional tensile testing. [1] Milkereit, Wanderka, Schick, Kessler, Materials Science and Engineering A 550 (2012) 87–96[2] Reich, Kessler, Materials Performance and

Characterization, 1 (2012) 1, DOI 10.1520/ MPC104632

11:20 AM Lunch Break

ICME Implementation and Case Studies

Tuesday AM
June 2, 2015

Room: Colorado III
Location: Cheyenne Mountain Resort

8:00 AM

Developing Refractory High-Entropy Alloys: Computation-Guided Experiments: *Michael Gao*[1]; J.W. Qiao[2]; B. Zhang[3]; H.W. Yao[2]; S.M. Guo[3]; S.Z. Yang[4]; C.S. Carney[1]; P.J. Jablonski[1]; J.A. Hawk[1]; D.E. Alman[1]; [1]National Energy Technology Lab; [2]Taiyuan Institute of Technology; [3]Louisiana State University; [4]Southern University and A&M College

High entropy alloys (HEAs) are potentially promising materials for applications in extreme environments because they have reduced chemical driving force towards degradation, sluggish diffusion, and good tensile strength at high temperatures. The presence of five or more principal components in equal molar ratios maximizes the configurational entropy and thus stabilize the solid solution phase. In principle, the more components that make up the solid solution phase, the higher the configurational entropy of mixing and the lower the free energy of the phase. This talk details a successful story in developing refractory HEAs integrating computation and experiments. The first step screening is done via the CALPHAD approach from a pool of 18 elements. A series of new promising HEA compositions are suggested that contain quaternary, quinary, senary, septenary and octonary principal elements. Model alloys down-selected from CALPHAD screening are then subject to first-principles density functional theory calculations, Molecular Dynamics simulations, and Monte Carlo simulations. Structural, thermodynamic, electronic, vibrational, and elastic properties are predicted. Guided by the computational predictions, experimental effort has been carried out in alloy fabrication, heat treatment, microstructure characterization using x-ray diffraction and electron microscopy, mechanical property characterization such as hardness and compression tests under ambient and high pressure, and high-temperature oxidation. In light of the present study, strategies in searching for new HEA compositions are presented, and HEA formation rules are discussed.

8:20 AM

ICME Based Accelerated Materials Innovation: *Jiadong Gong*[1]; David Snyder[1]; Jason Sebastian[1]; Greg Olson[1]; [1]QuesTek Innovations

ICME methodologies and tools have been developed and applied to the design of a series of novel alloys for customized properties to meet performance requirement in critical applications. Thermodynamic and kinetic models and databases for multicomponent systems have been developed that enable accelerated materials innovations. The successful computational development and implementation of QuesTek's Ferrium® M54 alloy validates the ICME approach in new materials design. On the other hand, application of ICME tools in the additive manufacturing front demonstrates improved efficiency and accuracy in process optimization and qualification, helping to accelerate the maturation of the additive technology in various alloy systems. Case studies of recent development in QuesTek Innovations highlights the role of ICME in the process design, validation and uncertainly quantification of the additive manufacturing of Ni, Al, and Ti based alloys.

8:40 AM

A Computational Framework for Designing g/g' Co-based Superalloys: *Shengyen Li*[1]; Eric Lass[1]; Daniel Wheeler[1]; Ursula Kattner[1]; Carelyn Campbell[1]; [1]National Institute of Standards and Technology

Co-Al-W-based g/g' (FCC_A1/FCC_L12)superalloys show promise as potential materials for aerospace turbine applications. The formation of a stable g/g' microstructure, similar to that used in the Ni-based superalloys, provides superior high temperature mechanical properties. Co-Al-W-Ta system is of interest because W contributions stabilize the γ' phase and Ta additions increase the solid solution hardening. To design a high performance superalloy (high UTS alloy at higher operating temperature) requires optimizing multi-dimensional space. This work proposes a computational framework that targets the composition and processing selections for high strength alloy. A genetic algorithm is used to construct the computational framework to determine potential compositions and corresponding processing conditions. The chemical composition and processing temperature path are selected as the initial inputs for the physical models. The γ stability of γ phase of the nominal composition at annealing temperature is evaluated using a Co-based multicomponent thermodynamic database. To determine the g-g' microstructure evolution as function of processing time the Avrami equation and LSW model are implemented. This analysis includes determination of the phase compositions and fractions and average g' size as functions of processing path. The average g' size distribution is used as input into a strengthening model. In order to evaluate the performance of the microstructure, the PyMKS (www.pymks.org) package is used to rapidly calculate the mechanical properties. The results are fed back to GAs and leading the selection of the inputs for next iteration. This framework provides efficient process to achieve the optimum solutions for this issue.

9:00 AM

Development of an ICME Approach for Aluminum Alloy Corrosion: *Kenneth Smith*[1]; Mark Jaworowski[1]; Rajiv Ranjan[1]; George Zafiris[1]; [1]United Technologies Research Center

Corrosion costs the United States over $1 trillion annually, yet is typically not analyzed at a detailed level during the product design phase. Our vision is to develop robust corrosion performance modeling tools that will ultimately enable us to predict corrosion behavior and generate composition-processing-structure-performance relationships that can be integrated into the product design standard work for product corrosion liability, and reduction of both the design cycle duration and cost. Our approach links modeling and experiments with verification and validation by coupling thermodynamic and kinetic modeling of alloy processing, phase-specific electrochemical characterization, and a multi-physics model description of the localized electrochemical properties such as corrosion current density. Material composition, processing conditions, and environmental exposure will serve as inputs to the predictive corrosion modeling. An initial application of this methodology on aluminum alloy will be presented and exemplary guidance on how the heterogeneity of the intermetallic (IM) particles within the alloy influence the alloy electrochemical response will be discussed. By understanding the phase-specific electrochemical response through measurements and density functional theory calculations, the impact of variations in alloy composition and processing can be related to the corrosion performance. Combining the intermetallic phase descriptions with the electrochemical response into a multi-physics model will then allow us to interrogate effects such as IM particles composition, size and distribution on the electrochemical response to guide alloy modification for corrosion risk mitigation.

9:20 AM

ICME and the Industrial Enterprise: Early Successes, Implementation, and Simplification: Katherine Stevens[1]; *Jeffrey Williams*[1]; Sanjay Sondhi[2]; [1]GE Aviation; [2]GE Global Research

As an industrial user and manufacturer of a broad range of engineering materials, GE has successfully applied ICME methodologies toward a number of aims including reduced material development cycle time, expanded exploration of materials and process design space, risk reduction for new technology implementation, and improved collaboration across technical disciplines. However, there remain challenges to continued expansion of ICME efforts particularly as models, software, experimental methods, data management solutions, and validation requirements grow in complexity. For example, GE has taken advantage of ICME for addressing challenges related both metallic and composite materials, but there at times has been a tendency to create silos of complexity around a given sub-discipline resulting in the need to deploy and maintain multiple models and/or tools. Creating an ever increasing number of models, tools, and characterization techniques may limit to overall effectiveness of ICME for an industrial enterprise and constrain opportunities for investment in new ICME approaches. Rather, as ICME matures, developers and practitioners must keep a focus toward simplification of the materials and process engineering function within industry.Examples will be provided of recent successes of materials modeling efforts and tool implementation that not only span multiple length-scales, and leverage a wide range of modeling approaches but also have been implemented in such a way that they have simplified the methods and practices for materials and process engineers within an industry setting. Additionally, challenges and opportunities for applying and maturing ICME approaches will be reviewed.

9:40 AM Break

10:00 AM

Adaptive Electronic Materials by Design: *James Booth*[1]; Nathan Orloff[1]; Darrell Schlom[2]; Craig Fennie[2]; [1]NIST; [2]Cornell University

Materials discoveries continue to drive innovation in electronics for future communications and computation systems. One example is provided by oxide material systems, which can potentially deliver many advantages for the development of low-loss, voltage-tunable devices for adaptive and cognitive electronics. We have used an integrated computational and experimental approach to design oxide material systems to deliver adaptive electronic behavior, identifying strained Ruddlesden-Popper phases of Srn+1TinO3n+1 as promising candidates for low-loss tunable microwave dielectrics. Ab-initio calculations demonstrate the emergence of a ferroelectric instability in these layered materials under biaxial strain, as a function of the layering index n, which provides a novel approach to tailor dielectric response in this material system. Synthesis of films with layering index n=2-6 with varying amounts of strain is accomplished using advanced deposition techniques, such as molecular beam epitaxy, and resulting samples are commensurately strained and display excellent structural properties. Dielectric measurements as a function of frequency, for a range of in-grown strains, temperatures, and electric-field bias, confirm ab-initio predictions of ferroelectric response for n>3 for samples grown with ~1% biaxial strain. Optimum performance at room temperature is achieved for strained n=6 samples, and this material forms the basis for the subsequent designs of high-performance tunable resonators and filters operating in the 10-40 GHz range. Feedback from device performance studies informs subsequent efforts in materials design and optimization. Our results illustrate the benefits of integrated computational/experimental approaches, which will be applied for further exploration of oxide materials for advanced electronics applications.

10:20 AM

Utilizing ICME models to More Effectively Predict Process-Structure-Property Relationships for Better Property Optimization and Design in Aerospace Alloys: *Ashley Goulding*[1]; Richard Neu[1]; [1]Georgia Institute of Technology

Precipitation-hardening is an important strengthening mechanism common in many aerospace alloys, with mechanical properties that can vary significantly as a function of traditional processing methods. Due to the multiple underlying physical mechanisms that are involved, the relationship between these properties and the processing methods can be difficult to accurately predict using computational models alone. Instead, the strategy taken here utilizes an ICME approach to develop process-structure tools independently of structure-property tools that can be effectively integrated to establish the process-structure-property relationships necessary for alloy design and optimization. Here, empirical computational tools, based on artificial neural networks, are used to link processing parameters such as quench rate, solution-, and heat-treatment to the microstructure characteristics such as grain size, percent recrystallization, and dispersoid and precipitate size and volume fraction, based on new experimental data generated on Al 7050 plate. Predictive computational models based on well understood physical mechanisms were developed to relate these microstructure characteristics to strength and fracture toughness. The strength model captures the influence of several strengthening mechanisms, including solution strengthening, precipitation hardening, and the influence of substructure. Fracture toughness is considered to be a combination of both intergranular and transgranular fracture, and is related to the degree of recrystallization, the grain boundary characteristics, and the strength of the grain interior. By integrating these vastly different tools, they can be used to facilitate the optimization of processing parameters and microstructures to achieve the best performance of a given alloy.

10:40 AM

Utilizing the Bond Bundle for Material Design: *Jonathan Miorelli*[1]; [1]Colorado School of Mines

The bond bundle, a topological feature of the charge density defined by the density's ridge structure, is a powerful utility for discerning the various bonding environments present in a material. The bundle, in principle, can be applied to any material or molecular system and thus there exist myriads of potential applications within material design. This talk will briefly cover a number of "success stories" involving the bond bundle. Such as using the bond bundle to discern the evolution of bonds across a Fe-ceramic interface which allowed for guided alloy design. The bundle was also successful in providing both a theoretical justification for the concept of a trigger linkage within explosive materials as well as revealing the role intra- and intermolecular effect have on the trigger linkage and thus explaining the differences between gas-phase and crystalline decomposition mechanisms in relevant energetic materials, such as in RDX. The usefulness of the bond bundle will be further elucidated by using it to compare Mo/Ta dislocation cores which have identical atomic configurations but different twinning anisotropies. The bond bundle in this case will reveal that the structure of the electron charge density is different and offers insight into why the antitwinning dislocation glide of Ta does not occur along the closest packed plane.

11:00 AM

ICME Support for Jumbo Vertical Bloom Continuous Caster: *Patrick Anderson*[1]; Krich Sawamiphakdi[1]; Dongbu Cao[1]; Christopher Eastman[1]; [1]TimkenSteel Corporation

In 2014 TimkenSteel commissioned a state of the art jumbo vertical bloom continuous caster at the Faircrest Steel Plant. This $200 million investment provides for additional capacity, manufacturing flexibility, superior cleanness for strand cast products, and broader capability to support higher value SBQ and seamless mechanical tube markets. In preparation for specification of caster design and material quality, computational modeling tools were applied to evaluate the anticipated product quality and variation from the existing process path. Process modeling included computational fluid dynamics modeling for design and operation of the tundish (alongside physical water modeling), deformation modeling of soft reduction roll effects on porosity and segregation, thermal modeling to evaluate transformation and thermal stress effects during cooling and reheating, and process modeling to ensure the identified metallurgical solutions fit within the practical manufacturing time envelope.

11:20 AM Lunch Break

ICME Models, Tools and Infrastructure II

Tuesday AM
June 2, 2015

Room: Amphitheater
Location: Cheyenne Mountain Resort

8:00 AM

Coupling Phase-field Modeling and Real Time Synchrotron X-ray Observation to Analysis the Influence of Cooling Rate on the Dendritic Morphology of Mg-Gd Alloys during Solidification: Yongbiao Wang[1]; *Liming Peng*[1]; Longqing Chen[2]; [1]Shanghai Jiaotong University; [2]Penn State University

The six-fold symmetry petaloid dendritic morphology of Mg-Gd alloys during solidification was demonstrated by using the phase-field simulating method combining with in situ synchrotron X-ray observation. As the cooling rate changed, the simulated solute profile ahead of solidification front in the liquid and the velocity of the SL interface changed accordingly, which were in fair quantitative agreement with real time synchrotron X-ray observing results. The process of directional solidification was also simulated. The modeling results show that different cooling rate produces different interface moving velocity, and introduces the transition from columnar to equiaxed grain growth during solidification (CET). Besides, by comparing the in situ observation, the phase-field model was modified more similar to the practical solidification, which has important meaning for predicting the microstructure evolution of Mg-RE alloys during solidification processes.

8:20 AM

Application of Machine Learning Techniques for Inverse Prediction in Manufacturing Process Chains: Sapan Shah[1]; Sreedhar Reddy[1]; Avadhut Sardeshmukh[1]; *BP Gautham*[1]; Gautam Shroff[1]; Ashwin Srinivasan[2]; [1]TRDDC, Tata Consultancy Services; [2]IIIT, Delhi

It is becoming increasingly widespread to use physics-based simulations of manufacturing processes. A goal of these simulations is to predict the properties of material or defects in a product. This often requires the solution to an "inverse problem" --- predicting inputs of the simulator from desired outputs. This task is usually ill-defined, and solved by formulating it as a constrained-optimization problem. Extensive simulation in the input-parameter space when performing the optimization is avoided through response surfaces constructed from results of simulations. In this paper, we report on the use of machine learning to address the inverse problem. Specifically, using data from physics-based simulations, we explore the use of two different kinds of models constructed by machine learning. The first is a purely predictive model, used in a manner analogous to a response-surface model, capturing complex non-linearities followed by the use of optimization for inverse prediction. For optimization, we used simulated annealing method. The second approach constructs a "generative" model (a Bayesian network), from which input values can be obtained directly from output values, without the need of an optimization step. It does however need additional knowledge in the form of conditional (in)dependences between process parameters, intermediate state variables, and outputs. We present results for modelling two processes: (a) a multistage wire drawing process; and (b) a heat treatment process chain involving carburization, quenching and tempering. In both cases, we find the generative model to be less effective and needs further investigation on aspects such as data sufficiency.

8:40 AM

Capturing and Transforming Phase-Based Materials Data: The Materials Data Curator: *Carelyn Campbell*[1]; Alden Dima[1]; Sharief Youssef[1]; Philippe Dessauw[1]; Guillaume Sousa Amaral[1]; Mary Brady[1]; [1]National Institute of Standards and Technology

An essential part of ICME is the ability to share and transform materials data among various computational tools. The NIST Materials Data Curator (MDC), a Python/MongoDB/Django Web-based system, provides a means for capturing, sharing, and transforming data. While the initial use case for the MDC is centered on phase-based property data, the MDC is designed to be a flexible general-purpose scientific data curation system. The data are organized using user-selected templates encoded in human and machine-readable extensible mark-up language (XML) schemas. These templates are used to create data entry forms that then generate XML documents to contain the data. The documents are saved in non-relational (NoSQL) database, MongoDB, via a two-way transformation that converts the XML documents into MongoDB's native BSON format for storage and back into XML during retrieval. The data can be searched and retrieved in a variety of ways: a template-driven Web-based form; a query-based tool, SPARQL; and an application-programming interface (API). The retrieved data can then be transformed into other formats as needed by different computational tools. The API also enables scientific workflow systems, such as Kepler and Taverna, to be integrated with MDC and facilitates federated searches of interconnected MDC repositories. The curation of various computational and experimental phase-base property data, including diffusivity, thermal expansion, molar volume and some phase equilibria data, will be demonstrated using the MDC. Using the search features, a variety of data sets will be combined and then used within a simple workflow tool.

9:00 AM

Facilitating the Selection and Creation of Interatomic Potentials (Force Fields) with Robust Modeling Tools and a New Data Infrastructure: *Zachary Trautt*[1]; Chandler Becker[1]; Lucas Hale[1]; [1]National Institute of Standards and Technology

The Materials Genome Initiative (MGI) seeks to significantly decrease the cost and time of development of new materials. Within the domain of atomistic simulations, several roadblocks stand in the way of reaching this goal. While the NIST Interatomic Potentials Repository (IPR) hosts numerous interatomic potentials (force fields), researchers cannot easily determine the best choice for their use case. Researchers developing new potentials, specifically those in restricted environments, lack a comprehensive portfolio of efficient tools capable of calculating and archiving the properties of their potentials. Additionally, students, the next generation of materials engineers, have limited access to fully functional and documented examples of production research using atomistic simulations. This talk provides a broad overview of work to date and plans to address these challenges within the IPR project. This talk will also highlight the benefits of adopting MGI infrastructure for materials data exchange.

9:20 AM

nanoHUB as a Platform for Implementing ICME Simulations in Research and Education: *Tanya Faltens*[1]; Alejandro Strachan[2]; Gerhard Klimeck[2]; [1]Purdue/ NCN; [2]Purdue

nanoHUB.org is an open access cyberinfrastructure that is supported by the National Science Foundation, and serves as a powerful and versatile platform for delivering computational resources to enable the implementation of Integrated Computational Materials Education (ICME) simulations in classroom settings. nanoHUB enables free cloud scientific computing, where users can access simulation tools for research and education using a web-browser or iPad, without the need to install software or have access to local computing resources. The tools have friendly, fully-interactive graphical user interfaces, meaningful default values, output of both numerical data and visualizations, and extensive support material that provides an accessible pathway towards advanced materials simulations. On the back end, nanoHUB computational resources include high performance computing clusters that enable research-quality simulation. The nanoHUB platform can be used to facilitate ICME in research and education in two distinct ways: by using existing tools or by creating and publishing new, customized nanoHUB tools. Existing nanoHUB tools are currently used to introduce simulations in ICME courses in a variety of areas such as electronic structures, diffusion kinetics, and mechanics of materials. These tools were created by installing the available open source code into nanoHUB, then building custom GUIs using the RAPPTURE toolkit, which is integrated into the nanoHUB workspace. In a similar manner, instructors can install other simulation tools into nanoHUB using RAPPTURE to easily customize their tools to meet their learning objectives. This presentation will introduce existing nanoHUB ICME tools and the procedure for customizing and publishing new tools on nanoHUB.

9:40 AM Break

10:00 AM

A Review of Materials Data Infrastructure Projects: *Scott Henry*[1]; Larry Berardinis[1]; [1]ASM International

Access to digital data and the ability to use data in an integrated computational materials engineering framework are key challenges for advancing materials and manufacturing innovation. Since the announcement of the U.S. Materials Genome Initiative in 2011, several initiatives have been launched to develop the resources and protocols necessary to support a robust materials data infrastructure. These projects have yielded promising results, and they have also helped to uncover and clarify the remaining issues and challenges. The ASM International Computational Materials Data Network has been an active participant in several of these projects – focusing on areas such as materials data management, a common vocabulary for online data interchange, and microstructure data – and also has been compiling an inventory and analysis of U.S. and international materials data infrastructure projects. This presentation reports on the status and initial outcomes from CMD Network projects and summarizes the scope, focus, and current status of government, commercial, and society initiatives. It proposes approaches for building upon these efforts to consolidate and further advance the materials data infrastructure needed to support ICME.

10:20 AM

Atomistic Simulations of Polymers in the Cloud: Resources for Research and Education: *Alejandro Strachan*[1]; Benjamin Haley[1]; Chunyu Li[1]; [1]Purdue University

Amorphous polymers and their composites are key engineering materials with applications ranging from structural components in aircraft to packaging in electronics. Predictive atomic-level simulations of these materials are highly desirable to provide constitutive laws and materials parameters for continuum simulations and to inform experimental design efforts. These simulations remain challenging and state-of-the-art methods are not widely available to the research and education communities. We will discuss our efforts to develop simulation tools for polymer simulations and make them universally available for cloud computing via NSF's nanoHUB. The framework under development consists of three main components: i) powerful simulation tools including state-of-the-art molecular builders, MD simulation stencils for structure relaxation and property characterization and post-processing codes; ii) a UQ framework to orchestrate the molecular simulations and propagate uncertainties in input parameters and explore trends; iii) databases of force fields and molecular structures as well as predicted and experimental properties.

10:40 AM

An Integrated Collaborative Environment for Materials Research: Mark Benedict[1]; *Matthew Jacobsen*[1]; Bryon Foster[1]; Charles Ward[1]; [1]USAF/AFRL

Commercial software and other tools developed in isolation from their actual users and use context have had a poor track record of supporting the complex computation and data flows that are essential to the practice of Integrated Computational Materials Science and Engineering. In fact, the increasing obsolescent and artificial separation of scientist from software developer actively impedes progress in creating communities of practice that share the burden of software and infrastructure development in order to reach pragmatic science and engineering driven goals. An overview will be provided on efforts to establish such a community of practice within a large materials research laboratory in order to develop an Integrated Collaborative Environment (ICE) that aids in materials and process discovery. The central challenge to implementing an integrated and federated system is in balancing the conflicting needs of insuring long term viability by utilizing software design best practices such as separation of concerns and component driven architectures, with immediacy of user needs for simple, flexible, autonomous and secure information management. Additionally, system behaviors modeled after an optimized research process must not impede the ability of practitioners to perform mission critical research. Key elements and design choices of the emerging ICE system will be presented in the context of a focused and requirements-driven use case that supports the digitization and curation of metallographic specimens and associated analysis.

11:00 AM

Computational Characterization of Network Structure and Nanovoid Growth of Thermoset Polymers: Chunyu Li[1]; *Alejandro Strachan*[1]; [1]Purdue University

Thermoset polymers have been extensively used as the matrix of fiber composites because of their high stiffness, high creep resistance and high thermal resistance. A fundamental understanding of the structural evolution and the relationship between material properties and molecular network structures is of great interests to the material community as well as aerospace industry. Recent years, we developed a thermoset simulator (MDPoS) to mimic chemical reactions in the curing process of thermosets. Thermo-mechanical properties of the crosslinked systems can be 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. Crosslinking degree and crosslink density are two important characteristics for amorphous thermoset polymers and they are related but not identical. Although great attention has been paid to their measurement by various methods, accurate determination of these characteristics is still a challenge for experimentalists. Most recently, we have developed a technique to characterize the detailed topology of network structure and nanoscale voids for establishing structure-property relationship. We will present our most recent progress in computational characterization of polymer network. The algorithm in our computational characterization will be described in detail. Our calculations indicate the network structures formed at different conditions could be very different even with the same crosslinking degree. The growth of nanovoids under mechanical loading is tracked and the percolation of void clusters is believed to be responsible for polymer yielding. Some material properties are shown more sensitive to the structure details.

11:20 AM

Uncertainty Quantification of Quantitative Structure-property Relationship Models of Composites: *Paul Patrone*[1]; Andrew Dienstfrey[2]; Stephen Christensen[3]; Samuel Tucker[3]; Andrea Browning[3]; [1]IMA; [2]NIST; [3]Boeing

In the composites industry, a key role of atomistic-scale simulations is to identify novel or previously untested, high performance cross-linked polymer systems. This task is complicated by the enormity of the design space, which arises from the fact that the large number of commercially available ingredients (amines and epoxies) can be combined in near limitless ways. In this work, we combine uncertainty quantification tools with reduced order modeling in order to identify a system and its mechanical properties on the basis of a few graph theoretic properties of its constituent monomers (molecular ingredients). Following a quantitative-structure property relationship (QSPR) approach, we map monomer chemistries to a few quantifiable metrics, e.g. the distance between bonding sites. Within the context of this low-dimensional parameter space, we then gather a limited set of simulated and experimental data points on mechanical properties, which we interpolate via Gaussian-process type tools. The end result is a response surface, with associated uncertainties, that maps structure properties of the monomers to mechanical properties of the associated bulk material. Importantly, this QSPR-type mapping provides a way to say which systems are "near" to one another in terms of performance, while quantifying the uncertainties associated with reducing complicated systems to just a few numbers. This enables computationally-informed material scientists to identify promising material systems and focus data gathering efforts only on those regions where uncertainties are high.

11:40 AM

PyMKS: A Tool for Modeling Microstructure/Response Relationships in Python: *Daniel Wheeler*[1]; David Brough[2]; Tony Fast[2]; Surya Kalidindi[2]; [1]NIST; [2]Georgia Tech

Microstructure informatics is an emerging field of study that encompasses techniques from signal processing, advanced statistics and data science. The Materials Knowledge System (MKS) (Kalidindi 2012, Fast 2011) forms an important subset of microstructure informatics by providing a localization technique to bridge the micro and macroscales. An MKS model is calibrated using established numerical models or experimental data at the microscale by calculating a set of influence coefficients using regression analysis. The influence coefficients are then scaled up to provide an approximate model at

the macroscale. A Fourier transform is used to both calibrate the coefficients and predict the response making the MKS highly efficient when compared to standard numerical models. The calibrate/predict MKS paradigm enables an existing inefficient physics-based code to provide approximate results at much longer length scales and relieves developers from focusing on efficiency issues when developing new physics-based codes.The PyMKS framework is an object oriented set of tools and examples written in Python that provides high level access to the MKS method enabling rapid analysis of microstructure/response relationships. The PyMKS uses the standard Python libraries making it work well with the existing scientific Python ecosystem. In particular, it relies on Scikit-learn for tuning sample sizes and hyperparameters. The presentation will provide an introduction to the MKS and an overview of the capabilities and implementation details of PyMKS.

12:00 PM Lunch Break

Plenary Session II

Tuesday PM
June 2, 2015

Room: Colorado II & III
Location: Cheyenne Mountain Resort

2:00 PM Invited
Integrated Computational Materials Engineering (ICME) of Generation Three Advanced High Strength Steels: *Louis Hector Jr*[1]; [1]General Motors

While traditional methods for materials development often involve laborious trial-and-error testing over protracted time frames, Integrated Computational Materials Engineering (ICME) is offering a means to significantly accelerate this process. Advanced high strength steels (AHSS), which contain multiple phases (e.g. ferrite, bainite, pearlite, austenite, martensite), and may exhibit phase transformation with strain, are fertile ground for ICME. However, prediction of macro-scale constitutive behavior based upon the multi-scale physical, chemical, and mechanical phenomena in these complex microstructures is a formidable challenge for ICME. Unprecedented collaboration between universities, industry, and government labs will be required to address AHSS development, curating of data, and the implementation of these materials into products that benefit the American consumer. We will begin with a brief overview of a DOE/USAMP-funded ICME program aimed at the development of Generation Three (Gen 3) AHSS. The lack of commercial Gen 3 steels that meet DOE targets is offering significant challenges to this ICME program. We will emphasize how the program is meeting these challenges following three thrusts: (1) production and testing of Gen 3 steel lab heats to DOE targets; (2) development of the ICME model which incorporates mutli-scale experimental and theoretical outputs into state variable constitutive models evaluated in forming simulations; (3) incorporation of the ICME model into vehicle performance simulations. The ability to manipulate material microstructures through the ICME model for the development of future Gen 3 steels will be discussed. The ultimate goal of converting the ICME model into a "UMAT" for CAE simulations will also be considered.

2:30 PM Invited
Integrated Computational Materials Engineering Approach to Automotive Lightweighting: *Kaan Inal*[1]; Raja Mishra[2]; [1]University of Waterloo; [2]General Motors R&D

Computational Materials Engineering tools capable of integrating microstructure based material and process design with performance driven structural optimization can play significant role in enhancing manufacturing competitiveness in future. Automotive industry is embracing ICME tools to adopt aggressive engineering strategies to meet impending fuel economy and vehicle mass targets through application of aluminum alloys in a sustainable manner. Computational tools that can aid the smart use of current materials and also accelerate the development of aluminum sheets with enhanced formability and surface quality or extrusions with enhanced crashworthiness are needed. This research presents multi-scale computational frameworks involving coupled micro-scale and macro-scale numerical models to guide upstream material and process development as well as downstream tool and manufacturing development for automotive component fabrication. For the micro-scale computations, a new 3D finite element analyses based on rate-dependent crystal plasticity theory is developed that incorporates 3D microstructures accurately constructed from 2D electron backscatter diffraction (EBSD) data into finite element analyses. Mechanism based constitutive laws that permit strain hardening and saturation without external adjustment are employed. The macro-scale computations are done with advanced yield functions informed by micro-scale models. Extended Finite Element Models (X-FEM) and Element Free Galerkin approaches are used. Coupling these models with optimization frameworks based on genetic algorithms and neural networks provide a comprehensive ICME tool set to satisfy design and performance requirements with materials and processes to meet cost, mass and performance requirements simultaneously. Examples of this integrated approach to develop aluminum sheets and extrusions will be presented.

2:50 PM Invited
Importance of Controlling Microstructure Heterogeneity When Designing Steel: *Kohsaku Ushioda*[1]; Hideaki Sawada[1]; Masaaki Sugiyama[1]; [1]Nippon Steel & Sumitomo Metal Corp.

Steels have many unexplored possibilities, and the elucidation and control of heterogeneity in microstructures, deformation, and dislocation behaviors are required to fully draw out their potential capabilities. The optimum design of materials processing and microstructures based on fundamental research is expected to achieve discontinuous improvement in their performance. In this paper, focus is placed upon the heterogeneity in the deformation structure of poly-crystal Fe, which is the most essential issue in thermo-mechanical processing. Heterogeneous deformation in grain boundary vicinities, shear bands, and deformation zones around particles significantly affects grain refinement and crystal orientation.Detailed experimental facts are presented followed by a discussion of the current situation and future works on the 3D CP-FEM calculation of heterogeneous deformation combined with the phase-field simulation of recrystallization and phase transformation. The kinetics of recrystallization and phase transformation are known to be affected by segregated alloying elements. Here, the retardation of austenite to ferrite phase transformation by the segregation of B in an austenite grain boundary is discussed from both experimental and calculation viewpoints. Moreover, the behaviors of deformation and fracture in Fe-Si alloy will be discussed in terms of dislocation behavior such as the double-kink formation in screw dislocation and the restriction of cross slip by the addition of Si. Although the discussion will be conducted from experimental and calculation perspectives, the change in the core structure of screw dislocation in the presence of Si should be fundamentally clarified. Finally, the future works are proposed for material integration.

3:10 PM Invited
ICME for Process Scale-up: Importance of Vertical and Horizontal Integration of Models: Gerald Tennyson[1]; Rishabh Shukla[1]; Saurabh Mangal[1]; Savya Sachi[1]; *Amarendra Singh*[1]; [1]Tata Consultacy Services

ICME will play a major role in reducing the lead time in development of a new product or component. One of the areas where ICME is likely to play a crucial role is process scale-up of mill products. Process scale-up of a mill product from laboratory to production stage is largely done through hit-and-trial and is a non-trivial exercise. It involves plant level trials which are expensive and time consuming. Use of ICME can significantly reduce the design search space and thereby bring down the cost and time of development. However many challenges need to be addressed to realize the full potential of ICME at an industrial scale. Manufacturing any product/ component involves a host of unit operations and the properties of the end product are intrinsically linked with final as well as intermediate processing steps. To link the material-processing-structure-performance matrix, there is a need to enhance models across various unit operations through multi-scale/multi-phase modeling and integration of models at various length scales. This allows for the information flow across various unit operations and thereby ensures horizontal integration of models. This step is crucial in designing set points and quantifying the influence of various unit operations on end product performance. In this paper, we illustrate the vertical-horizontal integration of models through an example.

3:30 PM Break

ICME Tools Showcase

Tuesday PM
June 2, 2015

Room: Colorado II & III
Location: Cheyenne Mountain Resort

4:00 PM Carl Zeiss X-ray Microscopy Inc.
4:10 PM MICRESS
4:20 PM ESI North America
4:30 PM Simpleware
4:40 PM Thermo-Calc Software
4:50 PM Materials Design Inc.

Poster Session II

Tuesday PM
June 2, 2015

Room: Colorado I
Location: Cheyenne Mountain Resort

PII-1: A Curve Swarm Algorithm for Global Search of State Transition Paths: *Lijuan He*[1]; Yan Wang[1]; [1]Georgia Institute of Technology

Atomistic scale simulation can predict state transition processes of materials such as adsorption, diffusion, and reaction. The challenge of the accurate prediction is to obtain a global view of many local minima and saddle points on the potential energy surface (PES) of a material system. The transition conditions are determined by the saddle points on the PES with the minimum energy barrier between local minima. In this paper, a new algorithm is developed to exhaustively search local minima and saddle points within a region of PES in order to provide a global view of the energy landscape. Unlike the existing saddle point search methods, the algorithm represents a transition path by a parametric Bézier curve with control points. It uses multiple groups of such curves, each of which represents a multistage transition path. During the searching process, each group of curves communicates with others to maintain cohesion and avoid collision based on a collective potential model. The algorithm is integrated with density functional theory calculation and demonstrated by diffusion of hydrogen atoms in the FeTiH system.

PII-2: A Quantized Crystal Plasticity Model for Nanocrystalline Metals: Connecting Atomistic Simulations and Physical Experiments: *Lin Li*[1]; [1]University of Alabama

Nanocrystalline (NC) metals, which consist of grains or crystallites with sizes less than 100 nm, have exhibited unique mechanical properties, such as extremely high strengths, very extended elastic-plastic transitions, and limited ductility, in comparison to coarse-grained counterparts. Such features pertain to their emerging deformation physics as grain size decreases into nano scale. One of the atomistic processes identified by molecular dynamics (MD) simulations is that a dislocation spontaneously transverses a nano grain interior after depinning from grain boundary ledges, producing a dramatic jump in grain-averaged shear strain. Inspired by this atomistic picture, a quantized crystal plasticity (QCP) model is developed to explore its connection to the unique NC mechanical features. The QCP model employs a crystallographic description of dislocation slip plasticity; in particular, single slip events across nano scale grains impart large (~1%) increments in grain-averaged plastic shear. Consequently, plasticity does not proceed in a smooth, continuous fashion but rather via strain jumps, imparting violent grain-to-grain redistribution in stress. Finite element simulations implementing the QCP model are not only able to capture the aforementioned unique NC features, but also reproduce the unique the trends in peak width evolution for NC metals measured by in-situ X-ray diffraction tests. Furthermore, the QCP model provides an insight into the activation spectrum of the atomistic events via bridging the disparity in length and time scales between MD simulations and physical experiments.

PII-3: An Interface to Quantum ESPRESSO: Linu Malakkal[1]; *Barbara Szpunar*[2]; Juan Zuniga[2]; Ravi Siripurapu[2]; Jerzy Szpunar[2]; [1]University of Saskatchewan ; [2]University of Saskatchewan

Our project aims at providing the materials engineering fraternity with a simple and effective interface using ipython to operate Quantum ESPRESSO (QE), an open source code for materials. QE is a first principles code using density functional theory, plane waves and pseudo potentials which has excellent ability to predict material properties. Ipython notebook interface uses the scope of the libraries including Atomic Simulation Environment (ASE), matplotlib, scipy, numpy, Elastic and newly developed libraries: QE-util-advanced to predict the properties. The complete exemplary notebooks with calculations, analysis and plots for various engineering applications using the initial version of QE-nipy, has been described on the following website http://homepage.usask.ca/~bas627/nipy/Nipy.htm. Recently we have developed the advanced version of the QE-nipy called QE_nipy_advanced which can take the full advantage of QE-code. In our latest version we have added features that can take care of all the input parameters supported by QE. The thermo-mechanical properties as a function of temperature for future nuclear materials such as Silicon Carbide, Beryllium Oxide, Uranium Carbide and Uranium Nitride have been studied. We acknowledge access to high performance supercomputers at CLUMEQ, West grid and Plato at the University of Saskatchewan and the initial developmental work by P. Jochym during his visit at the University of Saskatchewan. The previous similar developments of QECalc by Nikolay Markovskiy and Alexander DementsovThis work was mainly supported by grant from the National Sciences and Engineering Research Council of Canada

PII-4: Analysis of Published Cast Iron Experimental Data.: *Siddhartha Biswas*[1]; Charles Monroe[1]; Thomas Prucha[2]; [1]University of Alabama at Birmingham; [2]American Foundry Society

Material selection is always driven by multiple constraints. Tools available to a designer such as Ashby plots can be used to study the tradeoffs, such as density and stiffness, of various material systems. One class of materials, cast iron, has a rich history of property characterization over the last 200 years. In the cast iron system, the microstructure plays an important role in the final properties. In addition to chemistry, the microstructure of cast iron develops from process variables such as addition sequence, cooling rate, spherodizing treatment, inoculation treatment, hold time, etc. Full computational modeling of this material is elusive because of these process variables and spatial variations. Numerous works have been done in the past to control the microstructure to achieve desired cast iron. The purpose of this review is to compile and compare the historical experimental results. Important cast iron properties such as tensile strength, hardness, thermal conductivity are catalogued into a database from reported properties. This work should help gaps in experimental and modeling work to be more easily identified for future research programs.

PII-5: Applying Inverse Algorithm for In-Situ Resonance Inspection: *Kevin Lai*[1]; Wei Xu[1]; Xin Sun[1]; [1]PNNL

Resonance inspection (RI), which employs the natural frequency spectra shift between the good and the anomalous part populations to detect defects, is a non-destructive evaluation (NDE) technique with many advantages such as low inspection cost, high testing speed, and broad applicability to structures with complex geometry compared to other contemporary NDE methods. It has already been widely used in the automobile industry for quality inspections of safety critical parts. The authors have previously demonstrated an inverse algorithm that would quantify the flaw details, e.g. location, dimensions, and types. It is demonstrated that a variety of common structural flaws, i.e. stiffness degradation, voids, and cracks, can be accurately retrieved by this algorithm even when multiple different types of flaws coexist. However, the effectiveness of the inverse algorithm relies on an assumption that the frequency shift caused by flaws is significant higher than the discrepancies between parts. In this study, the effectiveness of the inverse resonance algorithm is discussed aiming at the noise to signal issue, and a modified inverse RI algorithm is proposed that will have in-situ advantage of the part, regardless of the initial discrepancies of the original parts.

PII-6: Benchmarking Multi-scale Models through Micro-mechanical Testing and Characterization of Ni-base Superalloys: *David Eastman*[1]; Zafir Alam[1]; Jessica Krogstad[2]; George Weber[1]; Somnath Ghosh[1]; William Lenthe[3]; Tresa Pollock[3]; Paul Shade[4]; Michael Uchic[4]; Kevin Hemker[1]; [1]Johns Hopkins University; [2]University of Illinois, Urbana-Champaign; [3]UCSB; [4]Air

Force Research Laboratory

Microstructure-dependent deformation models depend on both detailed structural characterization and constitutive properties, and require experimentally obtained benchmarks at salient length scales. Traditional methods for validating structural materials with bulk properties are a good start but miss many of the underlying microstructural details. In the current study, micro-mechanical tests of Ni-base superalloys have been designed and carried out in order to complement and support parallel multi-scale modeling efforts. Starting with bulk material, micro-scale samples and corresponding mechanical tests have been developed and are being used to elucidate the underlying microstructure-property relations for polycrystalline Rene 88. Employing these micro-scale experiments facilitates determination of both local and global properties. These experiments also allow for meso-scale characterization through collection of key features, such as grain size, grain orientation and local strain accumulation, for a finite number of grains that are tractable in crystal plasticity modeling. Connecting these explicit microstructures to their mechanical behavior captured through experimentation, and providing these results for modeling, opens a valuable pathway for model development and validation.

PII-7: Bondalyzer: A Tool for the Discovery of Charge Density Property Relationships: *Tim Wilson*[1]; [1]Colorado School of Mines

A great challenge of ICME is to relate the macroscopic properties of materials to their charge densities as obtained through ab initio calculations. The discovery of these relationships rests largely on our ability to describe inter- and intra-molecular bonding in a meaningful and consistent way. Built on the quantum theory of atoms in molecules, a bond bundle is the region of space around the topological bond path, from which bond-like properties can be calculated. Bond bundles are rigorously identified from topological features, specifically critical surfaces, of the electron charge density, and contain useful information such as bond electron counts. The geometry of the bundles and the forces exerted on their surfaces by the surrounding electron density provide new and valuable insight into the reactivity and other properties of the system. Bond bundles also exist for non-bonding and lone electron pair regions and help explain and categorize their significance. They have been used in the analysis of structural failures in ceramics, grain boundary propagation in ferrous materials, and trigger linkage in explosive compounds. They have also been used to provide a methodology for alloy improvement and design from first principles. Finding bond bundles, however, is a non-trivial computational task that has hindered their widespread adoption and utilization. Here we show examples of the use and application of a post-processing tool—codename Bondalyzer—for calculating, visualizing and analyzing bond bundles and other topological features in electron density fields with ease.

PII-8: Coarse-Graining Simulations of the Correlation between Free Volume Evolution and Plastic Deformation of Highly Cross-Linked DGEBA Polymer: *Amin Aramoon*[1]; Stephen Barr[2]; Timothy Brietzman[2]; Christopher Woodward[2]; Jaafar El-Awady[1]; [1]Johns Hopkins University; [2]Air Force Research Laboratory

Highly cross-linked polymer networks (e.g. epoxies) are widely used in many automotive, marine, and aerospace applications. Predicting the damage and failure of such systems is of crucial interest for their reliable performance. In this work, a coarse-grained Molecular Dynamics model has been developed to characterize the evolution of free volume density (voids) in DGEBA polymers under loading and its correlation to plastic deformation (e.g. hardening and failure). A detailed atomic monomer is coarsened to create the tailored plastic behavior. Cross-linked polymer networks are created under different curing conditions, including temperature, and cross-linker functionality using a dynamic cross-linking algorithm. The effect of chain size, and degree of cross-linking are also investigated. The free volumes are measured as a function of strain by fitting the largest ellipsoid between neighboring chains in the network. From these simulations we develop a direct correlation between the evolution of plastic deformation and the free volume density.

PII-9: Dimension Tolerance Analysis of Aluminum Casting Components: *Quan Zhibin*[1]; Zhiqiang Gao[1]; Qigui Wang[2]; [1]Southeast University, China; [2]General Motors Corporation

Aluminum casting components are usually subjected to heat treatment including quenching process. A significant amount of residual stresses and distortion can be generated during the quenching process. To evaluate whether the dimensions of the distorted casting component are still within the dimension tolerance of the final machined part, an efficient computational geometrical analysis algorithm has been developed by integrating nonlinear programming method with greedy algorithm. This paper will discuss in detail the formation of the problems and development of the greedy algorithm.

PII-10: Discrete Dislocation Dynamics Simulation of the Effect of Tension-Twins on the Plastic Deformation of Magnesium Crystals: Haidong Fan[1]; Sylvie Aubry[2]; A. Arsenlis[2]; *Jaafar El-Awady*[1]; [1]Johns Hopkins University; [2]Lawrence Livermore National Laboratory

Twining and slip are two important deformation mechanisms especially in hexagonal-close-packed (HCP) metals. Furthermore, the interaction between twin boundaries (TBs) and dislocations play an important role in the plastic behavior of HCP materials. In this work we present a new implementation of a twin boundaries (TBs) into the framework of DDD to simulate the collective evolution of dislocation and their interactions with TBs in magnesium (Mg) crystals. In addition, a nominal grain boundary (GB) model based on experimental results was introduced as well to mimic the GB's barrier effect. The model is then utilized to investigate the strong influence of (10-12) tension twins on the yield stress and hardening behavior of Magnesium. The, TB migration and the effect of twin volume fraction are fully characterized. Our simulation results show that TBs act as a strong obstacle to gliding dislocations, and contribute greatly to the hardening behavior of magnesium. On the other hand, the deformation accommodated by twinning plays a softening role. Therefore, the concave shape of the stress-strain curve comes from the competition between TB-induced hardening and twin-induced softening.

PII-11: Energy Landscape of \931-Grain Boundaries: The Space of Boundary-Plane Orientations: *Arash Dehghan Banadaki*[1]; Srikanth Patala[1]; [1]North Carolina State University

The structure of the grain boundaries (GBs) is a function of five macroscopic degrees of freedom, parameterized by the misorientation and the boundary plane orientation. In order to optimize the performance of polycrystalline materials by grain boundary engineering, it is necessary to investigate the structure-property relationships of GBs in the five-parameter space. We have calculated the energies of \931 3 GBs, for aluminum and copper, over a wide range of boundary plane orientations, elucidating the GB structure beyond the traditional twist and tilt boundaries. The simulations reveal a remarkably continuous evolution of GB structure resulting in a smooth energy landscape, which is free of cusps. Similar features are expected for misorientations corresponding to higher\931-values. Using this information, we will present a strategy to efficiently compute the five-dimensional GB energy landscape.

PII-12: MedeA® - an Atomistic Simulation Environment for ICME: *Paul Saxe*[1]; Clive Freeman[1]; Erich Wimmer[2]; [1]Materials Design, Inc.; [2]Materials Design, SARL

During the past 15 years the MedeA software environment has been adopted worldwide as the preferred tool for atomistic simulations by many leading industrial and academic research laboratories. MedeA includes comprehensive experimental structural databases (over 800,000 entries) and phase diagrams, sophisticated tools for the construction of atomistic models, for example grain boundaries and interfaces, and convenient analysis tools. With a fully integrated suite of leading simulation methods for ab initio, semi-empirical and classical simulations, namely VASP, MOPAC, LAMMPS and GIBBS, MedeA provides computed materials properties and atomic-level understanding for a wide range of systems including metal alloys, semiconductors, ceramics, organic polymers, fluids, and their interfaces. The MedeA environment harnesses the power of large-scale computing through a flexible three-tier software architecture driven by flowcharts that allow the development of complex, reproducible workflows. These workflows can call on any of the underlying building, computational and analysis tools and are increasingly being used with methods such as cluster expansion in UNCLE, or CALPHAD methods, in order to reach larger time- and length-scales. The capabilities of MedeA will be illustrated by examples highlighting the value of the range of methods and their integration. A discussion of standardization and a perspective on the combination of MedeA with mesoscopic and macroscopic simulation tools will conclude this contribution.

PII-13: Mesoscale Modeling of 3-d Voids Evolution in Large Ingot during Multi-hit Deformation: *Zhenshan Cui*[1]; Chao Feng[1]; Xiaoqing Shang[1]; Xinjia Li[1]; [1]Shanghai Jiao Tong University

Due to non-uniform solidification, internal void defects (like porosity and shrinkage) often exist in the large ingot and behave as sources of damage in the materials performance. Multi-stage forging process, like stretching swaging and upsetting, is often used to eliminate the voids. However, the material with voids inside often undertakes loading from different direction in different forging stage, which may results in closure-reopen effects of the voids. Therefore, modeling the 3-d deformation behavior of the voids is of great significance in multi-hit deformation of the ingot. A 3-d voids evolution modeling is presented by using mesoscale representative volume element (RVE). In the RVE, the deformation of the void is expressed as a function of the remote stress, remote effective strain-rate and the void aspect parameter. The coefficients of the model are determined from the finite element (FE) calculations of the RVE. In this model, the change of void radius is influenced by the mean stress and the deviatoric stress in the corresponding direction. The relationship between the void radius deformation rate and the void aspect parameter in the corresponding direction are heuristically established as inverse proportional functions. As a consequence, the volume and shape of the voids can be obtained by integrating the material deformation history. By combining the void evolution model with macroscopic finite element simulation of the multi-stage forging process, the voids evolution can be efficiently predicted and the condition for closing the voids can be obtained. This model is validated by laboratory experiments and applied in industry.

PII-14: Micromechanical Approach for R-value Prediction of Dual-phase Steel: *Jinjin Ha*[1]; Ji Hoon Kim[2]; Myoung-gyu Lee[3]; Frédéric Barlat[1]; [1]Pohang University of Science and Technology (POSTECH); [2]Busan National University; [3]Korea University

A microstructure-based FE analysis was carried out to predict the mechanical properties of a dual-phase (DP) steel. The FE simulations were performed using a representative volume element (RVE), which was obtained from real images of the microstructure. This RVE was constructed from 2D data obtained by serial sectioning (mechanical polishing) and converted into a full 3D volume. The plastic properties of each phase were described using a dislocation density approach coupled to empirical equations that are based on chemical composition. This FE model was applied to analyze the effect of microstructure on r-value and stress-strain evolution for materials subjected to non-linear strain paths. The results of these microstructure-based simulations were compared with those obtained using conventional or more advanced continuum models, including isotropic, kinematic and distortional hardening.

PII-15: Microstructure Design in LENS Manufactured Components: *Jacob Smith*[1]; Jian Cao[1]; Wing Kam Liu[1]; [1]Northwestern University

The Laser Engineered Net Shaping (LENS) process is a highly localized manufacturing process which utilizes a high-powered laser concentrated on metal powder material, either with the mass flowing into the focal point of the laser or selectively in a powder bed, in order to melt and solidify the powder. An accumulation of this melting and solidification process occurs in layers until a final component has been created. The benefit of this methodology is that extremely complex geometries can be created which are essentially impossible with other manufacturing methods. However, the highly localized nature of the process creates a particularly complex and interesting problem in that the microstructural characteristics are strongly based on the local process parameters, thermal history, and the component shape. Therefore, through careful process control the microstructure can effectively be designed to yield mechanical properties to satisfy specific criteria for design applications. The present work will discuss multiscale coupling techniques targeted at process parameter optimization for improved design of local microstructure characteristics of LENS manufactured components. The numerical techniques can further be implemented within a strict materials design framework to assist in selection intermediate iterations of the design process.

PII-16: Modeling and Experimental Verification of Fragmentation in Metal Alloys: *Doyl Dickel*[1]; Mark Horstemeyer[1]; [1]Mississippi State University

Understanding and prediction of fragmentation in metals has been a difficult problem in computational mechanics for many years. Due to the immense importance of fracture and damage on the microscopic scale to the eventual fragmentation of the macroscopic body, statistical models and internal state variable theory must be employed. The earliest statistical models give qualitative predictions of the size distribution of fragments, but rely on experimental results to provide the total number and mass of fragments. More recently, various measures of damage have been proposed to describe the total energy available for fragmentation. This energy can then be used to make predictions about the size and velocity distribution of the resulting fragments. In this presentation, a theoretical description of fragmentation is presented. Atomistic and continuum modeling of ballistic collisions are used to motivate the theory. From these results, predictions on the size and velocity distribution of fragments from a metal/metal impact are made. Predictions for the size distribution of fragments, including the total number of fragments produced, are then compared with experimental results from a high strain-rate impact test.

PII-17: Modelling the Microstructure of Polycrystalline Austenite-martensite Steels: *Alireza Rahnama*[1]; [1]Imperial College

A method based on the kinetics of crystal growth has been developed and applied to the computation of 3D microstrucuture in polycrystaline austenite-matensite steels. The detailed crystallography of the transformation and the effect of austenite grain size on the martensite-start temperature are employed to simulate a realistic martensitic microstrucuture. The interaction energy based on the plastic work model of Patel and Cohen is taken into account to model the variant selection under external system of applied stresses. The method has been integrated to the homogeneous deformation theory for computation of microstructure evolution in thermomechanical processing.

PII-18: Multiscale Modelling Platform: Smart Design of Nano-enabled Products in Green Technologies: J.P. Krugers[1]; D. Roosen-Melsen[1]; E. Coenen[1]; *Georg Schmitz*[2]; M. van den Brand[3]; T. Verhoeff[3]; O. Babur[3]; B. Patzák[4]; V. Smilauer[4]; G. Pacquaut[4]; M. Apel[2]; R. Altenfeld[2]; J. Olkkonen[5]; P. Myöhänen[5]; A.M. Lankhorst[6]; L. Thielen[6]; W.D. van Driel[7]; V. Hildenbrand[7]; J.M. Delgado Sanchez[8]; E. Sanchez Cortezon[8]; [1]TNO; [2]Access RWTH Aachen; [3]TU Eindhoven; [4]Czech Technical University; [5]VTT; [6]Celsian; [7]Philips; [8]Abengoa

The MMP project will develop an integrated modelling platform, especially equipped to target multiscale and multiphysics engineering problems. The innovation of MMP lies in its generic and modular concept, supported by data standardization and proper definition of application interfaces. This allows integration of existing simulation software and data repositories as plug-in components. The software platform developed in MMP will be distributed as open source software. This enables future users to join, contribute, and benefit from MMP. The versatility and power of the platform will be demonstrated by assessing two case studies on nano-enabled products with a high sustainability

impact. The performance of phosphor light conversion in LEDs and the efficiency of CIGS thin film processing for photo-voltaic devices will be increased. This presentation will summarize the objectives and the current status of the MMP project. It aims at a) Developing a Materials modelling platform b) Applying the platform concept to two different multiscale engineering problems (i)the performance of phosphor light conversion in LEDs and (ii)the efficiency increase of CIGS thin film processing for photo-voltaics devices MMP is supported by the European Commission under grant No. 604279Public website: http://www.mmp-project.eu/

PII-19: Optimization of a Platinum-nickel Surface by DFT Calculations: Emiliano Diez Tortorella[1]; Sandra Ulacco[1]; *Sandra Simonetti*[2]; [1]UTN; [2]UTN-UNS-CONICET

The development of modern theoretical surface science provides an opportunity to investigate structures on the atomic scale with useful applications in industrial technologies. From the technological point of view, bimetallic surfaces have recently attracted great attention by their activities as industrial materials in novel applications. Platinum and nickel are ones of the most versatile heterogeneous metals catalysis. Its chemical stability makes it a very convenient election in a lot of applications. In this work, a Pt-Ni(111) surface has been optimized with calculations carried out in the framework of the Density Functional Theory (DFT) using the Vienna Ab-initio Simulation Package (VASP). In this code plane wave basis sets are used to solve the Kohn–Sham equations. Electron exchange and correlation effects are described by the generalized gradient approximation (PBE). The electron–ion interactions are described by the projector-augmented wave (PAW) potentials. The fixed convergence of the plane-wave expansion was obtained with cut-off energy of 300eV. This value is based on a previous test, which calculation error was lower than 0.01eV. The two dimensional Brillouin integrations were full filled on a (3x3x1) Monkhorst-Packgrid previously tested. In order to evaluate the magnetic properties of the systems, the computations were performed at the spin-polarized level. The Pt-Ni(111) surface of FCC stacking layered structure was represented with a periodically repeated slab containing five layers of atoms separated in the normal direction by a vacuum region. The width of this gap was optimized to avoid the interaction between slabs. The lattice constants were also optimized.

PII-20: Performance Evaluation, Algorithm Optimization and Sensitivity Analysis of the Spectral Full-Field Deformation Modeling of Polycrystalline Materials: *Tugce Ozturk*[1]; Clayton Stein[1]; Reeju Pokharel[2]; Thom Popovici[1]; Franz Franchetti[1]; Robert Suter[1]; Anthony Rollett[1]; [1]Carnegie Mellon University; [2]Los Alamos National Laboratory

The Fast Fourier Transform (FFT) based full field deformation modeling technique is investigated via performance analysis tools TAU and CrayPAT in order to optimize the algorithm with respect to recent developments in high performance computing. Initial results from CrayPAT revealed that the code runs at less than desired peak performance, showing the necessity for optimization. To increase the performance, FFT calls, array indexing, LU decomposition and Newton-Raphson routines are investigated and optimized. TAU analysis tool, giving the per-function breakdown, allowed analysis of the parallelization performance, finding the scalability limit in parallelization, and minimizing communication overhead. For applications of the technique, it is useful to determine the smallest possible FFT representative volume element (RVE). Accordingly a sensitivity study is performed on a 3D High Energy X-Ray Diffraction Microscopy (HEDM) reconstructed Ni-based superalloy that contained a fatigue crack; the crack points to a hot spot in stress and/or strain. The test is also conducted on synthetically created 3D microstructures with anisotropy factors varying from 3.6 to 1.06, showing the sensitivity of the method to both elastic anisotropy and the number of grains per simulation domain.

PII-21: Probabilistic Occurrence of Weakest Link Microstructural Features in Two-Phase Titanium: *Joseph Tucker*[1]; Tyler Weihing[2]; Michael Groeber[3]; Adam Pilchak[3]; [1]Exponent, Inc.; [2]Southwestern Ohio Council for Higher Education; [3]Air Force Research Laboratory

A specific microstructural configuration has been identified as particularly damaging in terms of dwell fatigue crack initiation in two-phase titanium alloys. Specifically, this arrangement consists of neighboring "soft" and "hard" oriented microtextured regions (MTRs). MTRs are defined as clusters of alpha-phase titanium with similarly oriented [0001] axes. Routines were developed to quantify MTRs from electron backscatter diffraction data and these were implemented in DREAM.3D. Synthetic building algorithms were used to generate statistically equivalent datasets. These data were interrogated to determine the probability of occurrence of the dwell-fatigue-sensitive neighborhoods as a function of "hard" and "soft" definition (e.g. tolerance angle between stress axis and [0001] axis).

PII-22: Simulation of Microstructural Evolution of Three-dimensional Synthetic Microstructures during Deformation for Two-phase Titanium Alloys: *Sudipto Mandal*[1]; Anthony Rollett[1]; Shanoob Balachandran[2]; Dipankar Banerjee[2]; [1]Carnegie Mellon University; [2]Indian Institute of Science Bangalore

This work focuses on integrating various computational models and experimental tests in order to understand microstructure and texture development in near beta titanium alloys. Representative three-dimensional microstructures have been constructed based on experimental Electron Backscatter Diffraction (EBSD) data. An algorithm to examine preferential selection of variants from the EBSD data has been developed. It was observed that clusters of variants form in two-phase titanium alloys that share a common <111> direction in the beta phase parallel to a <11-20> direction in the alpha phase. A DREAM3D module would be developed to take into account the variants' information, habit planes, size and shape statistics from the experimental data when creating the synthetic microstructures. A viscoplastic self-consistent code is used to optimize the hardening parameters in order to match the experimental stress-strain behavior at different temperatures and strain rates. The deformation behavior of the synthetic microstructures is studied by observing changes in microstructure and texture using viscoplastic FFT codes using the optimized parameters. The effect of alpha phase morphology on the mechanical response would also be studied.This work is supported by the Boeing company.

PII-23: Study of the Influence of Heat Source Parameters and Build Profile on the Melt pool Dynamics in Additive Manufacturing: *Narendran Raghavan*[1]; Sreekanth Pannala[2]; Srdjan Simunovic[2]; Neil Carlson[3]; Sudarsanam Babu[1]; John Turner[2]; [1]University of Tennessee Knoxville; [2]Oak Ridge National Laboratory; [3]Los Alamos National Laboratory

Additive Manufacturing (AM), the fabrication of three dimensional parts from CAD model is expected to be a disruptive technology in transforming the manufacturing industry. Nevertheless, the highly transient phenomenon of heat transfer and fluid flow in the melt pool is poorly understood for the high temporal and spatial gradients occurring during the process. Hence, it is important to better understand the influence of the heat source parameters and unique build profiles on the melt pool dynamics in order to manipulate the microstructural evolution and control the mechanical properties of the part manufactured using AM. In this paper, influence of heat source parameters (beam diameter, spot on time, power, etc.) and build profiles (supported, unsupported, interfacial structures) on the melt pool dynamics of spot melting of stainless steel powder (SS 316L) using laser based AM process is studied. Effect of fluid convection inside the melt pool will also be reported by comparing pure thermal and thermal-fluid flow models. Truchas code developed by LANL (Los Alamos National Laboratory) is used to simulate thermal-fluid flow model of the process.Extensive analysis of the heat transfer and fluid flow patterns obtained as the result of the simulations will help in calculating solidification velocity and thermal gradient thereby correlating the input process parameters, build profile to the microstructural evolution. The results of the simulations will be validated with the experimental results. The detailed analysis of the simulations is also vital to reduce trials, improve process control, thereby reducing lead time for processing of new materials.

Plenary Session III

Wednesday AM
June 3, 2015

Room: Colorado II & III
Location: Cheyenne Mountain Resort

8:00 AM Invited
Integrated Computational Materials Engineering Needs for Aerospace: *James Cotton*[1]; RJ Glamm[1]; DM Rosenbladt[1]; E Pripstein[1]; S Christensen[1]; [1]Boeing

Low risk tolerance and long product cycles combine to make aerospace one of the most difficult industries to find benefit in integrated computational materials engineering (ICME) techniques. This challenge is exacerbated by a large product scale and a correspondingly large component scale, which lead to substantial kinetic differences between the laboratory and production. However, considerable needs persist for cost and weight reduction, and more critically, for accelerating the introduction of materials that enable such improvements. In this paper, we deconstruct the life cycle of aircraft materials and identify where ICME can offer substantial value. Several examples of the application of computational methods to aerospace materials problems will be presented, from exploratory material design, to scale-up simulations, to the estimation of damage tolerance properties, and for polymer and metallic systems. Finally, specific areas where ICME development is required will be highlighted.

8:20 AM Invited
Data Infrastructure Developed for PW-8: Nickel Base Superalloy Residual Stress Foundational Engineering Problem: *Terry Wong*[1]; V. Venkatesh[1]; Todd Turner[1]; [1]Aerojet Rocketdyne

The PW-8: Nickel Base Superalloy Residual Stress Foundational Engineering Problem is a program funded by the United States Air Force through the Metals Affordability Initiative (MAI) to address bulk residual stresses in Nickel-base superalloy engine disk components. These stresses can be induced during various manufacturing stages such as during the heat treatment process or the forging process. Bulk residual stresses can be a problem and result in component distortion during the machining process and/or during elevated temperature service. Bulk residual stresses are considered a Foundational Engineering Problem (FEP) that affects both suppliers and OEMs and is an issue that must be addressed with a cross-functional team. PW-8 addresses the problem of bulk residual stress in the manufacturing of a turbine disk by developing the infrastructure and tools needed to predict and incorporate bulk residual stress into the design and development of a turbine disk. In doing so, PW-8 answers the challenge given in a 2008 report issued by the National Academy of Engineering in which the authors commented that addressing FEPs are essential means to help establish the infrastructure needed to make Integrated Computational Materials Engineering a reality. This paper will report on a key aspect of the ICME infrastructure; namely the infrastructure needed to manage physical and model data. The paper will describe the data management infrastructure developed for PW-8, the lessons learned in this development and what can be applied to the ICME community as a whole.

8:40 AM Invited
Modeling and Simulation of Directional Solidification of Ni-Based Superalloy Turbine Blades Casting Assisted by Liquid Metal Cooling: Qingyan Xu[1]; Ning Tang[1]; *Baicheng Liu*[1]; [1]Tsinghua University

Turbine blades are the key parts of aero-engines and industrial gas turbines. In recent years, liquid metal cooling (LMC) is used in the directional solidification process to get higher temperature gradient and produce the large size blade casting. To reduce the developing cycle and cost, numerical simulation technology is used to predict the casting defects and optimize the LMC process.In this paper, mathematical models of directional solidification assisted by liquid metal cooling were established, including the heat transfer model which considered the heat convection between mold shell and cooling liquid metal, nucleation and grain growth model. The dynamic change of boundary conditions at different parts of the turbine blade casting was described. An additive gradient algorithm was proposed and developed to generate the mesh of mold shell with any smoothness that approximates to the real shell shape. Numerical calculation has been done for different LMC processes. The results show that higher withdrawing rate or lower cooling metal temperature led to higher temperature gradient and thinner mushy zone. If the withdrawing rate was too high, the mushy zone became concave. It is indicated that CET and freckle mostly tend to occur in the start part of the blade casting near the chill plate. Freckle also easily form at too low or too high withdrawal rate. Compared with conventional directional solidification, LMC process can prevent CET and freckle strongly and effectively. The numerical calculation results for freckle are in good agreement with those happened in a true SX aero-engine blade casting.

9:00 AM Invited
From Integrated Computational Materials Engineering to Integrated Computational Structural Engineering: *Rollie Dutton*[1]; Pam Kobryn[1]; Dale Ball[2]; James Castle[3]; Mark James[4]; Parviz Yavari[5]; [1]Air Force Research Laboratory; [2]Lockheed Martin Aeronautics Company; [3]Boeing Research & Technology; [4]Alcoa; [5]Northrup Grumman Corporation

Recent advances in the simulation of the quench, cold-work and machining processes for large aluminum forgings are opening the way for a new paradigm in the design, manufacture and sustainment of aircraft structures. The use of large forgings permits the unitization of smaller parts (brackets, fittings, lugs, etc.) with primary structural components like spars and bulkheads. This is being done in order to reduce part count, which in turn leads to significant reductions in manufacturing cost. Unitization can also translate into weight reduction / avoidance when comparing against built-up structure, but it raises a number of issues for structural durability and damage tolerance, notably reduced repair / replace capability and reduced crack arrest capability. The viability of the unitization concept is dependent not only on the availability of material systems that retain their mechanical properties in very thick sections, but also on the designer's ability to retain durability and damage tolerance, and to understand and mitigate the effects of residual stresses. Recently a "next-generation" design approach that directly addresses some of these issues has been developed and deployed. Among other things, this new approach requires the extraction of residual stress effects from material property data and the explicit re-introduction of those effects in selected, critical regions of the structure. In this paper we will provide an overview of an emerging application of ICME to the design of large aluminum forgings for aircraft primary structure and the concomitant development of verification and validation methodologies.

9:20 AM Invited
Preparing for the Future of Computing: Bridging Scales within the Exascale Materials Co-design Center*: *James Belak*[1]; [1]Lawrence Livermore National Laboratory

The advent of Advanced / Additive Manufacturing and the Materials Genome Initiative has placed significant emphasis on accelerating the qualification of new materials for use in real applications. Within these workflows lies both the engineering scale qualification through building and testing components at scale and full-scale modeling with integrated continuum computer codes and the materials scale qualification through revolutionary methods to non-destructively measure microstructure (3DXRD) and physics specific experiments coupled with meso-scale mechanics simulations of the same physics specific experiment using the same microstructure. This ICME process is one of the use cases that drives the Exascale Materials Co-design Center (ExMatEx). The goal of the Co-design Center is very analogous to the acceleration of new materials deployment within the MGI, rather co-design accelerates the deploying of laboratory concepts for future computer components to enable a productive exascale computer system. To enable better meso-scale understanding in the continuum models, ExMatEx is creating a direct coupling between the continuum integrated code and direct numerical simulation of the meso-scale phenomena. Here we review the ExMatEx project, its use cases.*PIs: Jim Belak and Tim Germann. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DEAC52-07NA27344 and supported by Office of Science, Office of Advanced Scientific Computing Research.

9:40 AM Question and Answer Period

10:00 AM Break

Process and Performance Modeling II

Wednesday AM
June 3, 2015

Room: Colorado
Location: Cheyenne Mountain Resort

10:20 AM

A General Simulation Technology for Forging with Considering the Evolution of Voids, Grains and Cracks: Xinjia Li[1]; Xiaoqing Shang[1]; *Zhenshan Cui*[1]; Chao Feng[1]; Dingqian Dong[1]; [1]Shanghai Jiao Tong University

For the heavy forgings which may weigh hundred tons, internal void, grain size and cracks are critical issues in assessment of the forgings' quality. Many models were developed for evaluating these issues in previous research. This work focuses on the overall integration of these models for simulation of hot forging process of large forgings, especially for the heads of nuclear power vessels. The volume change of the voids was modeled by using representative volume element (RVE), and the deformation of void was expressed as a function of incremental remote strain and stress. The dynamic recrystallization and static recrystallization was considered to simulate the grain evolution. The grain size and fraction of recrystallization was established as the function of temperature, strain and strain rate, in which the model parameters can be recognized from the material flow curves. For the initiate of fracture during hot forging, the effective critical strain was obtained by regression of the test results of thermal tensions, and expressed as function of temperature and strain rate. Meanwhile, a damage accumulation was formulated via Oyane's damage function, which considers the influence of strain and mean stress. With the software development, these models were integrated with commercial finite element code DEFORM and were applied for multi-stage forging process. Some multi-stage forging processes were simulated and tested, which showed a good coincidence in the results. A forming of head of nuclear power vessel was simulated, and according to the simulation results, the forming schedule is modified.

10:40 AM

A Method for Determining the Set Points of the Ladle, Tundish and Caster for Manufacturing a High Strength Steel Slab: *Rishabh Shukla*[1]; Ravikiran Anapagaddi[1]; Janet Allen[2]; Jitesh Panchal[3]; Farrokh Mistree[2]; Amarendra Singh[1]; [1]Tata Research, Development and Design Center; [2]University of Oklahoma; [3]Purdue University

To meet requirements emanating from environmental, safety, and competition, auto manufacturers are demanding improved performance and reduced defect levels from steel makers. The defects are dependent on the design of unit operations, and the processing conditions in the ladle, tundish, and the caster. To improve performance and reduce defect levels, steel makers need to design the process considering multiple unit operations. In this paper, we present a method to determine the design set points of ladle, tundish and casting operation to meet the desired properties of a cast slab, for a given input of molten steel to the ladle. The decisions associated with ladle, tundish and slab continuous casting unit operations are modeled using the compromise Decision Support Problem (cDSP) construct. Within the cDSPs, the required properties and tolerable defect levels for the continuously cast slab and available process window for ladle, tundish and continuous casting are specified. An inductive approach (upstream-downstream design method) is adopted for exploring the solution spaces of the three unit operations as an integrated whole. In this paper, the design set points obtained using this method for ladle, tundish and continuous casting of slab for different set of requirements is presented. The primary advantage of the proposed method is that it enables rapid exploration of the steel slab production process space. The proposed method is extensible and other downstream processes involved in manufacturing of a finished product from steel will also be integrated together.

11:00 AM

ICME for the Integrated Design of an Automotive Gear Considering Uncertainty: *BP Gautham*[1]; Nagesh Kulkarni[1]; Pramod Zagade[1]; Janet Allen[2]; Farrokh Mistree[2]; Jitesh Panchal[3]; [1]Tata Research, Development and Design Center; [2]University of Oklahoma; [3]Purdue University

While the materials community within ICME is focused on model development and integration across scales, the primary challenge from a design standpoint is the utilization of these models within product development. There are various types of uncertainties associated with the input parameters and the models themselves. These uncertainties are propagated as we integrate and generate process chains. Typically performance estimation at the end of such integrated process chains may have high degree of uncertainty. One challenge in ICME is to integrate the process models while managing various types of associated uncertainties such as input, parameter, model and propagated uncertainties, and to develop process chains which can be used in product development. In this paper, we introduce the Inductive Design Exploration Method (IDEM), that facilitates the exploration of the design space in an inductive manner and provides designers with a set of solutions relatively insensitive to uncertainty. We capture the effect of process parameters on evolving microstructure and the properties at intermediate stages, and link it to the final properties such as surface and core hardness and case depth. This information from all stages of the process including intermediate states predicted by the simulation is used in exploration of the design space. In this paper, we discuss the salient features of IDEM and illustrate its efficacy in developing heat treatment process chain for designing an automotive gear to the desired design specifications.

11:20 AM Break

11:40 AM

Gamma Prime Evolution during Processing and Heat Treatment of the Nickel-Based Superalloy IN738LC.: *Magnus Anderson*[1]; Andrew Rowe[2]; Jonathon Wells[3]; Hector Basoalto[1]; [1]University of Birmingham; [2]RWE npower; [3]Siemens Industrial Turbomachinery Limited

Understanding the evolution of the intermetallic phase gamma prime in nickel-based superalloys is fundamental in the development of predictive theories of deformation. Composition and thermo-mechanical histories strongly influence the volume fraction, size distribution and morphology of gamma prime, as well as, its thermodynamic instability (leading to rafting and coarsening). Predicting such behaviour requires detailed models of the relevant physics which includes the influence of elastic interactions between particles and the overlapping of diffusion fields. Such modelling capability is desired to allow the prediction of location specific properties resulting from manufacturing and how these microstructures influence the integrity of components during in-service conditions. This paper focuses on the development of a multi-scale description of multimodal particle distributions and its evolution in nickel based superalloys during heat treatment. Mean field theoretical approaches have been very successful in describing the evolution of various aspects of the microstructure. However, such approaches need to be supplemented with additional information if they are to be extended to include nucleation of the gamma prime particles. Predictions from classical nucleation theory have been found to capture observed behaviour qualitatively however lack quantitative accuracy. Cluster Dynamics is a mean field description based on Lattice Kinetic Monte Carlo and offers an alternative approach to classical nucleation theory. This work presents a theoretical extension of cluster dynamics to large time scales representative of heat treatments and in-service conditions. Thus, the proposed approach provides a link between cluster nucleation and growth to the classical regime of particle coarsening described by LSW kinetics.

12:00 PM

Investigating the Influence of Microstructural Features on Strength and Ductility of Beta Annealed Ti-6Al-4V: *Matt Kasemer*[1]; Euan Wielewski[1]; Romain Quey[2]; Paul Dawson[1]; [1]Cornell University; [2]École des Mines de Saint-Étienne

Deformation and heat treatment processes can be used to alter an alloy's microstructure and in turn greatly modify the alloy's macroscopic properties like strength and ductility. Ti-6Al-4V is a dual phase alloy that exhibits a large amount of microstructural variability dependent on the thermomechanical processes it undergoes during manufacturing. At elevated temperature, this alloy is in its BCC (beta) phase. Annealing at this temperature results in a complex network of lamellar planes throughout grains of the primary HCP (alpha) phase upon cooling to room temperature. We discuss a parametric study - utilizing simulations based on a crystal-scale finite element formulation - in which the effect of variation of the microstructural parameters which describe beta annealed Ti-6Al-4V are determined. Data used to inform the instantiation of representative microstructures have been gathered by groups at Cornell, Carnegie Mellon University, University of California Santa Barbara, and The Ohio State University as part of a wider collaborative project. Aspects of the complex geometry of the microstructure, strength of texture, and the presence of a second crystallographic phase are studied in order to better understand the link between the microstructure and the bulk behavior of the material. Specifically, a distribution of strength is desired in order to provide a lower-bound estimate of strength for design purposes. The study also provides insight into the differences between the beta annealed microstructure and others that arise in Ti-6Al-4V.

12:20 PM

Multiphysics Modeling and Simulation of Electromagnetic Pulse Welding: *Wei Xu*[1]; Dangxin Wu[1]; Xin Sun[1]; [1]Pacific Northwest National Laboratory

Electromagnetic pulse welding (EMPW), as an innovative high-speed material processing technique that employs electromagnetically driven high-velocity cladding to achieve material joining, has been increasingly favored to accommodate the application of lightweight materials in the automotive industry. However, since various concurrent phenomena including excessive plastic deformation, material mixing, localized heat generation, recrystallization, and micro-cracking, etc. that can strongly affect the quality of the weld are generally involved within the process, further development and deployment of the EMPW technology requires a unified theory to comprehensively understand all these underlying mechanisms as well as their couplings. In the present study, the entire EMPW process has been investigated in an integrated multiphysics computational framework, where individual constituent sub-models to resolve different essential characteristics, i.e. electromagnetically induced dynamics, interfacial mechanics and kinetics were hierarchically developed and consolidated so that a quantitative correlation of the weld strength in terms of the operational parameters can be established. With good agreement found between the prediction and the experimental measurements, the proposed model is expected to help elucidate and shorten the technology improvement cycle.

12:40 PM

Through-process Modeling for Alloy Design and Process Optimization for Cold Spray Processing: *Danielle Belsito*[1]; Baillie McNally[1]; Victor Champagne[2]; Richard Sisson[1]; [1]Worcester Polytechnic Institute; [2]U.S. Army Research Laboratory

Military aircraft that require high maneuverability, durability, ballistic protection, repairability, and energy efficiency need structural alloys with low density, high toughness, and high strength. The cold spray process, a dynamic powder consolidation technique, produces materials that meet these needs. A through-process model was developed to be utilized as a predictive tool to design optimum aluminum alloys and processing parameters for the cold spray process. The four stages in the through-process model are powder production, powder preparation, cold spray processing, and post-processing. Each stage is a stand-alone model with the stages integrated to create a model of the entire cold spray process. This paper emphasizes the extensive computational thermodynamic and kinetic modeling employed to aid in novel material design of the powder. Model predictions are compared with experimental microstructure, microchemistry, and mechanical properties.

1:00 PM Lunch Break

Modeling at Different Scales III

Wednesday AM
June 3, 2015

Room: Colorado III
Location: Cheyenne Mountain Resort

10:20 AM

Calibrated Localization Relationships for Polycrystalline Aggregates by using Materials Knowledge System: *Yuksel Yabansu*[1]; Surya Kalidindi[1]; [1]Georgia Institute of Technology

Multiscale modeling of material systems demands novel solution strategies to simulating physical phenomena that occur in a hierarchy of length scales. Majority of the current approaches involve one way coupling such that the information is transferred from a lower length scale to a higher length scale. To enable bi-directional scale-bridging, a new data-driven framework called Materials Knowledge System (MKS) has been developed recently. The remarkable advantages of MKS in establishing computationally efficient localization linkages (e.g., spatial distribution of a field in lower length scale for an imposed loading condition in higher length scale) have been demonstrated in prior work. In these prior MKS studies, the effort was focused on composite materials that had a finite number of discrete local states. As a major extension, in this work, the MKS framework has been extended for polycrystalline aggregates which need to incorporate crystal lattice orientation as a continuous local state. This extension of the MKS framework for elastic deformation of polycrystals is achieved by employing compact Fourier representations of functions defined in the crystal orientation space. The viability of this new formulation will be presented for several case studies involving single and multi-phase polycrystals.

10:40 AM

An Efficient Hybrid 2D/3D Discrete Dislocation Dynamics Simulation for Engineering Dislocations Structures in Thin Films: *Siavash Sarrafan*[1]; Ray Fertig[1]; [1]University of Wyoming

Crystalline thin films are increasingly used in semiconductor devices, ferroelectric and ferromagnetic devices, biomedical components, fuel cells, solar cells and wear-resistant coatings. Substantial research has been devoted to attempting to understand how dislocation structures evolve and how they affect device properties. Dislocations that naturally arise during thin film deposition can result in deleterious effects at the device application level. Previous research has shown that by controlling deposition conditions dislocation densities can be tailored. Our recent work has shown that the dislocation structure itself has the potential to be controlled by applying an external strain during deposition. Current dislocation simulation methods are unable to predict this because they are too computationally intensive to model high dislocation densities, interactions, and their resultant deformations that are observed in some real applications.In this paper, we propose a novel method to exploit the quasi-two-dimensional nature of three-dimensional dislocation loops in a thin film to model their behaviors. For most film configurations, simulation performance can be enhanced by implementing a hybrid two-dimensional/three-dimensional model without losing significant fidelity. In this technique, misfits stress fields are modeled by superposing multiple two-dimensional models. Threads are modeled with a more traditional three-dimensional implementation as they move through the misfit stress field. Combining the two–dimensional and three-dimensional analyses, leads to a sizeable reduction in the computational costs. Consequently, much higher strains and/or dislocation densities can be studied. It is anticipated that this model will enable engineering of dislocation structures in thin films for specific device properties.

11:00 AM

Computational Modeling and Experimental Characterization of Martensitic Transformations in NiCoAl for Self-Sensing Materials: *Terryl Wallace*[1]; Vesselin Yamakov[2]; Jacob Hochhalter[1]; William Leser[1]; James Warner[1]; John Newman[1]; Ganga Purja Pun[3]; Yuri Mishin[3]; [1]NASA Langley Research Center; [2]National Institute of Aerospace; [3]George Mason University

Fundamental changes to aero-vehicle management require the utilization

of automated health monitoring of vehicle structural components. A novel method is the use of self-sensing materials, which contain embedded sensory particles (SP). SPs are micron-sized pieces of shape-memory alloy (SMA) that undergo transformation when the local strain reaches a prescribed threshold. The transformation is a result of a spontaneous rearrangement of the atoms in the crystal lattice under intensified stress near damaged locations, generating acoustic waves of a specific spectrum that can be detected by a suitably placed sensor. The sensitivity of the method depends on the strength of the emitted signal and its propagation through the material. The signal strength depends strongly on the SP shape and size and the crystalline microstructure characteristics, such as the size and orientation of the grains. The modeling effort employs molecular dynamics and Monte Carlo atomistic simulations together with finite element modeling at the particle level with developed SMA constitutive models. The atomistic simulations are performed with a recently developed embedded-atom interatomic potential to study the effect of chemical composition and uniaxial mechanical stresses on the martensitic phase transformation in NiCoAl alloys. The predicted martensitic transformations are compared to experimental data obtained from NiCoAl arc-melted buttons of various compositions. The simulated lattice parameters are within the 4% range of deviation from the experimental values, and the martensitic transformation can be reproduced well in the scattering range of 20% of the experimental data.

11:20 AM Break

11:40 AM

A Progressive Damage Model for Ceramic Matrix Composites with Processing-Induced Residual Stress: *Lucas Hansen*[1]; Anthony Waas[1]; [1]University of Michigan

Fiber-reinforced ceramic matrix composites are a promising material class for high temperature applications. A key mechanism in the behavior of these material systems is crack deflection, which allows the accumulation of damage in an otherwise extremely low toughness material. Cracks deflection is made possible by relatively thick fiber coatings. The relative compliance and weakness of the coatings prevents the continuation of matrix cracks into the fiber, allowing fiber bridging to occur. A method is presented to predict the progressive damage response of these materials, taking into account the effects of the thick coating as well as residual stress induced during manufacturing of the coupons or parts. Using a fracture mechanics based approach, the nonlinear response of the composite is predicted, including the effects of fiber pullout and friction. A key aspect of this model is the explicit inclusion of the fiber coating. It is shown that other approaches, in which the coating is either represented with a "homogenized coated fiber" or neglected entirely incorrectly predicts the stress distribution in the material, which leads to an incorrect response prediction, especially in the case of very thick fiber coatings.

12:00 PM

Effect of Interface Dislocation Recovery on the Strain-hardening Rate of the Nanolayered Metallic Composites -- An Atomistically Informed Interface Dislocation Dynamics Investigation: *Shuai Shao*[1]; Jian Wang[1]; Caizhi Zhou[2]; [1]Los Alamos National Laboratory; [2]Missouri University of Science and Technology

Owing to the high interface-volume ratio, the nanolayered metallic composites have shown unprecedented levels of strengths, ductility and damage tolerance in extreme environments. The interface acts as a special medium in which the defects can move, recover, nucleate, emit, or be absorbed. For instance, recent experiment on the Cu-Nb nanolayeres has provided evidence of interface dislocation recovery by observing constant level of interface dislocation density with increasing plastic strain. Interface dislocation recovery has direct impact on the nucleation rate of lattice dislocations and is therefore expected to significantly influence the strain-hardening rate of the composite. Atomic-scale modeling is able to reveal unit process (involving single or a few defects) occurring at interfaces during deformation with respect to kinetics and energetics, but is limited to time-scale (ns) and length-scale (nm). Current state-of-the-art micro-scale, meso-scale, and continuum scale modeling works well for micro-scale materials because of the dominated deformation processes by dislocation activities in phases. However, the interface physics is largely missing in those models. We are developing a new materials modeling tool at micro-scale by combining atomistic studies with the DD simulation – in accounting for the roles of interfaces on storage, recovery, nucleation, emission of dislocations within/at/across interfaces and their correlation with interface structures and properties. Here we report the development of the model as well as its application in the effect of interface dislocation recovery on the strain-hardening rate of Cu-Nb nanolayers.

12:20 PM

From Melt Pool to Strength - Application of ICME Methods for the Development of Rapid Manufacturing Technologies: *Tobias Maiwald-Immer*[1]; Thomas Goehler[1]; Andreas Fischersworring-Bunk[1]; [1]MTU Aero Engines AG

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 start with the 2D melt pool simulation for an SLM (selective laser melt-ing) process. The mapping to a 3D structure using equivalent heat sources is demonstrated and validated. The precipitation kinetics are calculated for the temperature-time history of the process and subsequent heat treatment using Caphad based methods. In a last step first prediction of the strength based on the precipitation condition is presented.

12:40 PM Lunch Break

ICME Models, Tools and Infrastructure III

Wednesday AM
June 3, 2015

Room: Amphitheater
Location: Cheyenne Mountain Resort

10:20 AM

CALPHAD Modeling and Microstructure Investigation of Mg-Al-Sn-Ca/Sr Systems: Weihua Sun[1]; *Alan Luo*[1]; [1]The Ohio State University

Previous research has shown as-cast Mg-Al-Sn ternary alloys offer good balance of mechanical properties. The present work extends the compositions with additions of Ca and Sr. Based on literature review and CALPHAD modeling, Mg-Al-Sn-Ca and Mg-Al-Sn-Sr quaternary alloys are prepared using an induction furnace and the phase constituents are investigated by X-ray diffraction and microstructural analysis. The microstructure is compared with the solidification simulations under equilibrium and Scheil conditions. The results not only supplement phase equilibria information of the Mg-Al-Sn-Ca/Sr systems, but also can assist alloy design and development in these systems.

10:40 AM

The Inverse Phase Stability as a Constraint Satisfaction Problem: *Richard Malak*[1]; Edgar Galvan[1]; Sean Gibbons[1]; Raymundo Arroyave[1]; [1]Texas A & M University

The development of new materials must start with understanding their phase stability. In the context of alloy design, the use of thermodynamic databases based on the CALPHAD approach have enabled the calculation of phase equilibria as a function of thermodynamic conditions such as pressure, composition, temperature. While useful, this is essentially a forward approach: given a set of thermodynamic conditions, obtain the resulting phase constitution (i.e. equilibrium) state. In the context of materials design, a much harder problem is that of mapping a desired region in the multi-dimensional phase constitution space to a set of corresponding thermodynamic conditions. Previously, other researchers have used optimization schemes to identify specific conditions that yield a particular phase stability state (e.g. minimum liquidus), essentially doing a point-to-point mapping. Here we focus on a more general problem: that of mapping specific hyper volumes in the phase constitution space to corresponding volumes in the thermodynamic condition space (set-to-set mapping). In the context of search theory, this type of problem is categorized as a Continuous Constraint Satisfaction Problem (CCSP). CCSP are extremely challenging to solve and here we present a highly novel framework combining computational materials science (i.e. Gibbs energy minimization), evolutionary computation and machine learning to solve CCSPs related to Inverse Phase Stability. While previously we have demonstrated the approach in relatively simple problems, here we apply the framework to investigate cases in which the system must be subject to (a priori) unknown sequence of thermodynamic conditionsto achieve specific phase constitution states.

11:00 AM

Modeling the Formation of Eutectic Castings: *Oriane Senninger*[1]; Peter Voorhees[1]; [1]Northwestern University

Directionally solidified ceramic eutectic in situ composites are candidates for high temperature structure materials. Indeed, the large area of eutectic phase interfaces can deflect cracks and thus generate excellent mechanical properties in industrial materials at high temperature. Mechanical properties in eutectic alloys are thus largely controlled by the alloy microstructure, in particular by eutectic colony size and the spacing of the phases within the eutectic. These microstructural properties are dependent on the solidification process. By controlling the eutectic solidification process one can thus optimize macroscopic mechanical properties. Performing this optimization by simulation can reduce significantly the time and cost of new materials development in industry. However, although models currently exist to simulate dendritic grain growth in industrial casting conditions, there is to our knowledge no such model for simulating eutectic grain growth in complex temperature fields. We propose here a new tool to model the growth of multiple eutectic colonies during solidification on the scale of a casting, by coupling a phase field model for eutectic growth with heat flow. In this model, the eutectic colony growth is assumed to grow isotropically, as opposed to dendrites which growth according to preferential crystallographic directions that are the basis for the well known CAFÉ models. The temperature field is coupled to eutectic colony growth using Jackson-Hunt theory. The veracity of our model is assessed by comparing the microstructures generated in our simulations with those obtained from casting experiments. The results of the model and comparison to experiment will be presented.

11:20 AM Break

11:40 AM

Predictive Simulation of Diffusion in Ni-based Alloys using Pair Interaction Model Based Kinetic Monte Carlo Method: *Dominic Alfonso*[1]; De Nyago Tafen[2]; [1]National Energy Technology Laboratory - DOE; [2]National Energy Technology Laboratory / URS Corporation

Investigation of diffusion processes in Ni-based alloy is a problem of high relevance in the area of understanding corrosion behavior. We explored the use of a combined approach consisting of density functional theory to compute migration barriers and kinetic Monte Carlo method to evaluate hard to measure diffusion coefficients in alumina forming Ni based alloys. A major challenge in the implementation is the need to find one by one the rate constant for each diffusion process that can happen in the alloy. To overcome this, a pair interaction model was utlized to evaluate the influence of the local environment on the kinetic parameters. The computational tool yielded Ni self diffusion coefficients in good agreement with experiments. The predicted Fe, Al and Cr tracer diffusion coefficients also compare well with previously reported experimental data. Al and Fe alloying elements were found to have a dragging effect on the mobility of oxygen. Incorporation of H atom into the Kinetic Monte Carlo framework will be discussed.

12:00 PM

Thermodynamic and Diffusion Mobility Modeling of the Aluminum-Hydrogen-Nickel-Oxygen System Augmented by First-principles Techniques: *Austin Ross*[1]; Xuan Liu[1]; Greta Lindwall[1]; Huazhi Fang[1]; Zi-Kui Liu[1]; [1]Pennsylvania State University

The incorporation of data predicted from first-principles during modeling of materials' thermodynamic properties by means of the CALPHAD (CALculation of PHAse Diagrams) method has proven to be powerful numerous times in recent years. In this work, the aluminum-hydrogen-nickel-oxygen (Al-H-Ni-O) system is in focus with emphasis on the solubility of H and O in the face-centered cubic (fcc) phase. The Ni-H, Ni-O and Al-O systems are remodeled to incorporate interstitial mixing information from density functional theory which enhances the physical meaning of the model parameters and consequently, increases the understanding of the energetics in the fcc phase. This is important when predicting its stability in relation to other phases in the Al-H-Ni-O system, such as different oxides. Calculations are also performed to predict the interaction of O and H in the Ni lattice and good agreement with extrapolations from the modeled binary systems is concluded. Additionally, the diffusion mobilities of H and O in the fcc phase are modeled by accounting for kinetic Monte Carlo data which allow for prediction of the composition and temperature dependency of the diffusion coefficients for H and O.

12:20 PM

Effect of Dislocation Density and Crystal Size on Surface Roughness Evolution under Cyclic Loading in FCC Metals from Discrete Dislocation Dynamics Simulations: *Ahmed Hussein*[1]; Jaafar El-Awady[1]; [1]Johns Hopkins University

Surface roughness evolution due to subsurface dislocation activity is one of the main triggers for crack nucleation under cyclic loading. In this work, we present large scale three-dimensional physics-based discrete dislocation dynamics (DDD) simulations to study crystal size-effects and dislocation density effects on the surface roughness evolution in FCC Nickel crystals. Simulation results of crystal sizes between 250 nm to 20,000 nm and spanning two orders of magnitude are discussed. In DDD, the dislocation microstructure is evolved in time under the applied load, and individual dislocations are tracked as they move and escape from the crystal surfaces. The displacement fields of the escaping dislocations are calculated and the resulting surface roughness due to surface steps remaining after dislocations escape is accurately quantified. Detailed results of the surface roughness evolution, stress-strain response, and dislocation density evolution, as a function of number of cycles are presented. Further insights on subsequent crack initials are discussed.

12:40 PM Lunch Break

Applications IV

Wednesday PM
June 3, 2015

Room: Colorado II
Location: Cheyenne Mountain Resort

2:00 PM

An Integrated Surrogate Modeling Approach for Materials and Process Design: *Melanie Senn*[1]; [1]Fraunhofer IWM

We propose an integrated surrogate modeling approach for the efficient design of materials and production processes. The proof of concept is shown by application to a phenomenological draw bending model that describes the relation between the process parameters (Young's modulus, Poisson's

ratio, blank geometry, coefficient of friction, blank holder force and punch velocity) and the spring-back as the process result. The introduced concept can also be applied directly to experimental data while taking into account the process noise as uncertainty (e.g. for process control). The integrated approach combines three components: design of experiments (DoE), surrogate modeling (based on function approximation by regression, e.g. artificial neural networks) and optimization of process or material parameters. DoE allows an efficient selection of experimental or simulation data to create a continuous and fast surrogate process model. The process model is used to determine the optimal (material or process) parameters w.r.t. a desired result (in this case minimum spring-back). The estimated parameters enable to rapidly find the optimal operating conditions for real experiments or to constrain them for further detailed simulation studies. We have evaluated and compared different designs, regression models and optimization procedures. Our results show that we obtain the same optimal process parameters for minimum spring-back from a detailed design (243 samples) as from a reduced design (81 samples). Future work involves applications to more complex experiments or simulations to efficiently determine the optimal process or material parameters by a sparse data sample that can be created with little cost.

2:20 PM

Uncertainty Management in the Integrated Realization of Materials and Components: *Janet Allen*[1]; Jitesh Panchal[2]; Farrokh Mistree[1]; Amarendra Singh[3]; BP Gautham[3]; [1]University of Oklahoma; [2]Purdue University; [3]Tata Research, Development and Design Center

We contend that ICME is not limited to selecting an available material from a database; instead, ICME includes actually tailoring material structure at various levels of hierarchy (atoms, microstructure, etc.) via associated processing paths to achieve properties and performance levels that are customized for a particular application. Accordingly, from a systems design perspective we view ICME as the top-down driven, simulation-supported, decision-based design of material hierarchy to satisfy a ranged set of product-level performance requirements. George Box is reputed to have said that all models are wrong but only some of them are useful. Form a systems design perspective we observe that in model-based realization of engineered systems, the decision maker must be able to work constructively with decision models and analysis models that are typically incomplete and inaccurate. Hence, the need to manage uncertainty. In this paper, we highlight our approach for managing uncertainty in the realization of engineered materials and components and a key development that is necessary to institutionalize ICME in industry, namely, a computational platform.

2:40 PM

Analysis of Strengthening in AA6111 during the Early Stages of Aging: *Alban de Vaucorbeil*[1]; Ross Marceau[2]; Gang Sha[3]; Simon Ringer[3]; Warren Poole[1]; [1]University of British Columbia; [2]Deakin University; [3]University of Sydney

Due to its good combination of formability and strength, the aluminum alloy 6111 is a popular candidate for automotive applications. Its strength is obtained by artificial aging during the so-called paint bake cycle. However, natural aging that occurs at room temperature beforehand can have, for medium to high strength alloys (i.e. Mg + Si > 1 wt.%), a deleterious effect on the subsequent increase in yield stress during the paint bake cycle. This is due to solute redistribution and clustering occurring during natural aging. In order to develop a structure-property model for strengthening during natural aging, atom probe tomography experiments were used to quantitatively determine the evolution in the composition, size and shape of solute clusters for different aging conditions. The size distribution of these clusters has been mapped onto the glide plane and then, using an areal glide model where the dislocation–obstacle interaction strength has been assumed to be related to the obstacle size on the glide plane, the stress necessary for a dislocation to pass through the range of obstacles has been estimated.It is demonstrated that the contribution of cluster strengthening during artificial aging at higher temperatures is dominated by the high number density of small clusters (radius <1 nm), whereas the situation during room temperature natural aging is more complex. The resulting yield stress model for cluster hardening can now be implemented into an integrated computational materials engineering model for property variation during processing of 6xxx aluminum alloys used in automotive applications.

3:00 PM

The Materials Commons: A Novel Information Repository and Collaboration Platform for the Materials Community: *Brian Puchala*[1]; Glenn Tarcea[1]; Emmanuelle Marquis[1]; Stravya Tamma[1]; John Allison[1]; [1]The University of Michigan

Critical to accelerating the pace of materials science and development is the development of new and improved infrastructure providing a seamless way for materials researchers to share and use materials data and models. To address this need, we are developing the Materials Commons, an information repository and collaboration platform for the metals community in selected technical emphasis areas. We envision the Materials Commons becoming a continuous, seamless part of the scientific workflow process. Researchers will upload the results of experiments and computations as they are performed, automatically where possible, along with the provenance information describing the experimental and computational processes. By associating this data with the experimental and virtual computational materials samples from which it is obtained, the Materials Commons will build process-structure-property relationships enabling the construction and validation of constitutive and process models. The Materials Commons website provides an easy-to-use interface for uploading and downloading data and data provenance, searching and sharing data. At its core, the Materials Commons consists of a secure data storage cluster, an application for efficiently uploading and downloading large data sets, and a REST based API to access and extend the capabilities of the repository. The API allows for features such as automated data upload from experiments and computations, seamless integration of computational models, and algorithmic analysis of process-structure-property relationships. The Materials Commons is a central thrust of the Center for PRedictive Structural Materials Science (PRISMS).

3:20 PM Break

3:40 PM

Use of Molecular Dynamics and Quantum Methods in Aerospace: *Sam Tucker*[1]; [1]Boeing

Numerical analysis methods such as FEM and CFD have been in use by Boeing for many years. Now Boeing is using atomistic and quantum level simulations to spearhead materials R&D efforts. These methods have been adapted to assist in solving problems related to in-service airplane operations and in the discovery of improved materials for future aircraft. Currently, atomistic MD is used to predict the thermal and mechanical responses of potential polymer candidates for use as paints, sealants, coatings, and matrices in fiber-reinforced composites. MD is also used to study fluid sensitivity and transport properties of materials. Quantum methods are used to predict polymer properties such as resistance to UV degradation and to study the reaction mechanisms of polymerization. Boeing is interested in expanding molecular modelling capabilities to facilitate faster and more nimble materials R&D.

4:00 PM
Effects of Heterogeneities on Recrystallization Kinetics and on Mechanical Properties of Partially Recrystallized Copper: Experiments and Modelling: *Fengxiang Lin*[1]; Yubin Zhang[1]; Dorte Juul Jensen[1]; [1]Technical University of Denmark

Creating a partially recrystallized microstructure is a possible strategy to increase the ductility of nanostructured heavily deformed metals. Two important questions for this strategy are: how the microstructure evolves during recrystallization and how the microstructural evolution affects mechanical properties. Following the general idea of ICME: that experimental data are used to deduce modeling tools, which then serve to predict effects of various processes, we address the two questions by both experimental characterizations and modeling of recrystallization microstructures and mechanical properties for two heavily deformed copper samples: one deformed by cold-rolling (CR) and the other by dynamic plastic deformation (DPD). The deformed microstructure of the latter sample is more heterogeneous. Based on the microstructural characterizations of a series partially recrystallized samples using electron backscatter diffraction, we developed a multi-stage recrystallization model. The recrystallization model predicts the kinetics in both samples well. For modeling the mechanical properties, uniaxial tensile tests were performed for both samples annealed to various fractions of recrystallization. A model using isostrain assumption was proposed to correlate the recrystallization microstructures to the mechanical properties. This model predicts well the mechanical properties for CR samples with various fractions of recrystallization. Less good agreement is however obtained for the DPD samples possibly due to the local strain heterogeneities, which will be considered in a next version. Together the two models would serve as a good ICME platform for evaluating effects of annealing on the mechanical properties of highly strained materials.

4:20 PM
A Continuum Dislocation Dynamics Approach to Crystal Plasticity of Two-phase Titanium Alloys: *Hector Basoalto*[1]; Jeffery Brooks[1]; [1]University of Birmingham

A requirement of current continuum descriptions of plastic flow is to capture the governing physics of dislocation motion and interactions between themselves and the material microstructure. This is fundamental in the development of predictive location specific property models that can be implemented within an integrated computational materials engineering framework. This paper will present a macroscopic description of plasticity that couples crystal plasticity and continuum theory of dislocations. In particular, field equations for the dislocated crystal are presented and the Nye dislocation density tensor is expressed in terms of microstructural parameters describing a two-phase alloy. Relations for self and latent hardening are also derived. The approach is applied to the modelling of the high temperature flow stress behaviour of titanium alloys with duplex and lamellar microstructures. It will be shown that there is a good agreement between predicted theoretical results with experimentally measured flow stresses for the alloy titanium-6Al-4V.

Modeling at Different Scales IV

Wednesday PM
June 3, 2015

Room: Colorado III
Location: Cheyenne Mountain Resort

2:00 PM Invited
PRISMS: An Integrated Predictive Multi-Scale Capability for the Materials Community: *John Allison*[1]; Larry Aagesen[1]; Samantha Daly[1]; Krishna Garikipati[1]; Vikram Gavini[1]; Margaret Hedstrom[1]; H. V. Jagadish[1]; J. Wayne Jones[1]; Emmanuelle Marquis[1]; Brian Puchala[1]; Shiva Rudraraju[1]; Veera Sundararaghavan[1]; Sravya Tamma[1]; Glenn Tarcea[1]; Katsuyo Thornton[1]; Anton Van der Ven[2]; [1]The University of Michigan; [2]University of California-Santa Barbara

Development of integrated multi-scale modeling capabilities linked with experiments will be necessary for efficient development of future ICME capabilities. This talk will provide an overview of the Center for PRedictive Integrated Structural Materials Science (PRISMS) which has as its primary mission the development of a unique scientific platform for enabling accelerated predictive materials science. We are developing and will make available to the materials community, a suite of open-source integrated multi-scale computational tools for predicting the microstructural evolution and mechanical behavior of structural metals. The integrated multi-scale computational tools being developed include software for statistical mechanics, real-space density functional theory, phase field, crystal plasticity and continuum plasticity, as well as software for integrating these codes and results from other advanced computational methods (e.g. dislocation dynamics) into a holistic capability. These computational methods are being tightly linked with advanced experimental methods for determining model inputs, filling gaps in theory and for validation. These advanced experimental methods include quantitative transmission electron microscopy and atom probe tomography, micro-digital image correlation and specialized in-situ fatigue experiments. This integrated capability is being demonstrated by providing improvements in the quantitative and predictive understanding of magnesium alloys, in particular precipitate evolution and the influence of microstructure on monotonic and cyclic mechanical behavior. An important element of the PRISMS Center is the development of "The Materials Commons," a knowledge repository and virtual collaboration space for curating, archiving and disseminating information from our experiments and computations as well as providing a collaborative platform and repository for the broader materials community.

2:20 PM Invited
Bottom-up and Top-down Uncertainty Quantification of bcc Fe Single Crystal Plasticity: *Aaron Tallman*[1]; Joel Blumer[1]; Yan Wang[1]; Sankar Narayanan[1]; Ting Zhu[1]; David McDowell[1]; [1]Georgia Institute of Technology

Two single crystal plasticity models of bcc Fe are used in combination to examine the flow rule for crystal viscoplasticity at the scale of individual phases/grains. The temperature-dependent and stress-dependent coordinated kinkpair activation energy considered from bottom-up atomistic simulations in terms of parameters in a thermally-activated flow rule. The top-down form of the flow rule introduces non-Schmid coefficients to model available experimental data from laboratory specimens across a range of temperatures. Uncertainty quantification is approached in two ways; parametric uncertainty is gathered through determination of confidence levels for parameter values, and model form uncertainty is approximated by a comparison of the output of the two models. Generalized interval probability theory is employed. The issue of how a mesoscale model can accept information from both bottom-up and top-down pathways is considered and discussed.

2:40 PM
Phase-Field Simulations of Precipitation in an Mg-Nd Alloy: *Larry Aagesen*[1]; Shiva Rudraraju[1]; Ellen Sitzmann[1]; Vicente Araullo-Peters[1]; Emmanuelle Marquis[1]; Katsuyo Thornton[1]; John Allison[1]; [1]University of Michigan

Precipitation hardening is an important strengthening mechanism in many magnesium-rare earth alloys. In these systems, plate-like precipitates are observed to form on prismatic habit planes. Such precipitates are very effective at blocking dislocations gliding in the basal plane, the predominant mechanism of slip in magnesium. The PRISMS phase-field code, a highly scalable parallel code based on the deal.II finite element library, has been developed for simulating microstructural evolution and is used to study the evolution of metastable beta-prime precipitates in an Mg-Nd alloy. The effects of site saturation conditions versus concurrent nucleation and growth are compared, and the effect of varying nucleation rate is considered. The morphology and size distribution of precipitates from simulation are compared to experimental results obtained using transmission electron microscopy and atom probe tomography. This phase-field code and integrated experimental-computational study are part of the Center for PRedictive Structural Materials Science (PRISMS).

3:00 PM
A Multi-Scale Comparison of Grain Boundary Structure Using the Phase-Field Crystal Model and Molecular Dynamics: *Jason Luce*[1]; Bradley Hodge[2]; Philip Goins[2]; Elizabeth Holm[2]; Katsuyo Thornton[1]; [1]University of Michigan; [2]Carnegie Mellon University

The phase-field crystal (PFC) model is emerging as a promising tool for quantitatively predicting material properties and behavior. One of the strengths of the PFC model is that it is capable of maintaining atomic scale resolution while still being able to describe phenomena that are observed at diffusive time scales. As such, the PFC model serves as a bridge between atomistic models, like Molecular Dynamics (MD) and mesoscale models, and thus could be integrated into an ICME framework. A key step in the parameterization of the PFC model is the verification of its ability to produce equilibrium atomic-scale structures. A recent PFC formulation by Greenwood et al. [1] has led to models that are capable of producing stable 2-D and 3-D structures based on phenomenologically derived two-body direct correlation functions (DCFs). This approach was used to generate 2-D grain boundaries for grains with varying degrees of misorientation. These grain boundary structures were then compared against those generated by MD simulations. A comparison of the equilibrium atomic positions in the two models show that there is good agreement in the grain boundary structure. [1] Greenwood et al., PRL 105, 045702 (2010)

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Additive Manufacturing of Two-Phase Titanium Alloys: A Micro-Macro Scale Modelling Approach: *Yogesh Sovani*[1]; Chinnapat Panwisawas[1]; Richard Turner[1]; Jeff Brooks[1]; Hector Basoalto[1]; [1]University of Birmingham

Additive manufacturing has rapidly become a widely used repair method due to the flexibility of adding features to cast, forged or machined parts without replacing the whole component. Selective laser melting is one of the additive manufacturing technologies, whereby a laser beam selectively melts successive layers of powder in a prescribed path by adding material layer-by-layer to allow a three-dimensional structure to be constructed. A multi-scale modelling approach has been developed to predict: (i) the microstructure formed during the process and (ii) the corresponding mechanical response. A computational fluid dynamics model has been used to simulate the interaction between the laser beam and representative spherical powder particles. During the subsequent cooling, the grain distribution is predicted using a finite element cellular automata model. The mechanical response of the material is then determined through a microstructure-informed crystal plasticity approach, which is able to account for variations in microstructure resulting from different cooling rates and predict the scatter in flow stress behaviour. The modelling results are critically compared with experimental data.

4:00 PM

Computation of Effective Radiative Properties of Powders for Selective Laser Sintering Simulations: *Daniel Moser*[1]; Sreekanth Pannala[2]; Jayathi Murthy[1]; [1]University of Texas at Austin; [2]Oak Ridge National Laboratory

Selective laser sintering (SLS) is an additive manufacturing technique for rapidly creating parts directly from a CAD model by using a laser to fuse successive layers of powder. Continuum models of the process require material properties such as laser absorptivity and laser extinction coefficient. In this paper, we determine these quantities computationally, and unlike previously published work, account for finite bed depth and polydisperse particulate distributions. We develop a Discrete Element Model (DEM) developed and implement it in the open source solver MFiX. An empty domain is initialized and particles are placed randomly at the top of the domain. They fall under the influence of gravity, interact with each other via a spring-dashpot model and finally settle. Once settled, rays are fired downwards into the particle bed from a random location at the top of the domain. They are absorbed and reflected by the particles until their energy is adequately diminished or they exit the domain. The effective absorptivity is then obtained by the ratio of the sum of the total energy absorbed by all the particles to the total energy input by the laser. The extinction coefficient is obtained by measuring the amount of energy that is able to penetrate to various depths in the bed. Results are compared against previous computational and experimental measurements for free, monodisperse powder beds and good agreement is obtained. Correlations along with uncertainties are developed to allow the effective absorptivity and extinction coefficient to be accurately set in SLS macroscale models.

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An Image Based Finite Element Model for Ni-Based Superalloys Using a Two Scale Constitutive Model: *George Weber*[1]; Somnath Ghosh[1]; David Eastman[1]; Will Lenthe[2]; Kevin Hemker[1]; Tresa Pollock[2]; Chris Woodward[3]; [1]Johns Hopkins University; [2]University of California, Santa Barbara; [3]U.S. Air Force Research Laboratory

A polycrystalline crystal plasticity finite element model (CPFEM) is developed for γ-γ' nickel-based superalloys with constitutive behavior established over two length scales. A dislocation density-based crystal plasticity model, at the scale of sub-grain microstructures containing γ' precipitates in the γ-matrix, is homogenized to yield a grain-scale activation energy-based crystal plasticity model. The two phase γ-γ' sub-grain structure is morphologically characterized by electron microscopy and statistically quantified in the model. The homogenized single crystal model is experimentally validated with single crystal tests. The single crystal constitutive model is incorporated into a micromechanical image-based CPFEM model polycrystalline RVE. To acquire a polycrystalline representation, Ni-based superalloy samples are serially sectioned by a focused ion beam and scanned with electron backscatter diffraction to incorporate experimentally accurate structural and crystallographic features into the model. A description of lattice incompatibility, grain orientation and grain structure is needed for this scale. Image-based CPFE model generation techniques are implemented to link experimental realizations of microstructural distributions to the mechanical material response. Complexities of the microstructural data are handled by developing integrated tools and algorithms which promote a transition from experiment to simulation without comprising the integrity of the data. At each length scale, benchmark experimental mechanical tests are designed to precisely measure local and global quantities for rigorous model validation and comparison. Constant strain rate and creep simulations are experimentally validated and connect the microstructural texture from material processing with the resultant mechanical response.

4:40 PM

Electric Field and the Kinetics Characteristics of the Growth of a Metal Oxide Film at High Temperature - Insights from Diffuse-interface Modeling and Simulation: *Tian-Le Cheng*[1]; You-Hai Wen[1]; Jeffrey Hawk[1]; [1]National Energy Technology Laboratory

The electric field developed during metal oxidation plays an important role on the kinetics and mechanism of oxidation. For high temperature oxidation at different length/time scales when the oxide film thickness grows up from nanometers to microns and above, the effect of the electric field on oxidation kinetics also changes. Here we present a novel oxidation model based on a diffuse-interface approach. It explicitly describes the gas/oxide/metal phases and incorporates interfacial reactions, mass diffusion, charge interactions, and moving boundaries. The metal-oxide interface is considered as an electrode-electrolyte interface in electrochemistry. By the scaling feature of the model the smooth transition of oxidation kinetics over a wide span of film thickness is captured. The essential characteristics of the electric field and its effects on oxidation kinetics at different length scales are discussed.

ICME Models, Tools and Infrastructure IV

Wednesday PM
June 3, 2015

Room: Amphitheater
Location: Cheyenne Mountain Resort

2:00 PM

HPC in Experiment-Informed Materials Genome and Materials Design: *Wing Liu*[1]; Jacob Smith[1]; [1]Northwestern University

Successful materials design as part of the materials genome initiative has indicated on numerous occasions the necessity of organizing and processing extremely large datasets obtained via experimental means. There have been recent attempts to incorporate these large datasets into numerical methods in order better understand the coupling between material microstructure and mechanical performance. These large datasets heavily motivate the need for improved High Performance Computing (HPC) techniques in order to obtain sufficient resolution for multiple scale modeling applications. The present work is directed at disseminating some of the complexities in correlating mechanics with large experimental datasets for materials characterization design. Applications for additive manufacturing, specifically the Laser Engineered Net Shaping (LENS) process, using SS316L as well as for other advanced alloys will be discussed. The underlying physical mechanisms governing the fracture process of these materials are taken into account by both higher-order continuum theories combined with advanced microstructure embedding techniques.

2:20 PM

High-Throughput Study of Phase Transformations and Microstructure Evolution using Diffusion Experiments: Changdong Wei[1]; Qiaofu Zhang[1]; Siwei Cao[1]; *Ji-Cheng Zhao*[1]; [1]The Ohio State University

This talk will summarize recent progress in studying phase transformations and microstructure evolution using high-throughput diffusion experiments. Diffusion couples and diffusion multiples are employed to create wide compositions of solid solutions through high-temperature thermal interdiffusion. Subsequent processing of the diffusion samples via continuous cooling or isothermal annealing at lower temperatures leads to various phase transformations. The resultant atlases of microstructures across wide composition ranges provide systematic information on the phase transformation kinetics. These atlases of morphologies are used to test and validate theoretical models in a much more effective and systematic manner than gathering information from individually made alloys. Examples will be used to illustrate the diverse applications of such diffusion experiments as part of the experimental approaches for ICME.

2:40 PM

Phase-field Simulations of Aluminization of Nickel-based Alloys during Pack Cementation: *Stefan Poulsen*[1]; Ashley Paz Y Puente[1]; Dinc Erdeniz[1]; Thomas Philippe[1]; Peter Voorhees[1]; David Dunand[1]; [1]Northwestern University

Aluminization by pack cementation is a well-known method to confer corrosion resistant diffusion coatings to Ni-based alloys. In the process, Al is deposited on the alloy surface by vapor phase deposition, creating an Al-rich coating. Subsequent inwards diffusion of Al results in a series of phase transformations such as Ni(Al)/Ni3Al, and Ni3Al/NiAl. This process thus involves diffusion of multiple elements through multiple phases, where the diffusivity is known to vary by several orders of magnitude between phases and with composition, making it a significant modeling challenge.We have investigated this problem with a quantitative phase-field model, i.e. a model which may employ physical parameters, thus removing the need for fitting model parameters to known data a posteriori. We employed CALPHAD optimized free energy functions and interdiffusion mobilities given by CALPHAD-style optimized assessments to simulate microstructural evolution during aluminization of Ni-Cr alloys. We present simulation results both for thin wires (d~200 microns), and for contact regions in woven meshes of such wires, where the detailed morphology of this intrinsically 3D structure has been determined by X-ray tomography, and simulation results are compared to experimental data. Since the code has been verified by experiment, it is now possible to use this to design new Ni-base alloys by varying the alloy composition and processing paths.

3:00 PM

Phase Field Modeling Of Recrystallization In Titanium-Aluminum Alloys: *Susan Gentry*[1]; Anna Trump[1]; John Allison[1]; Katsuyo Thornton[1]; [1]University of Michigan

Integrated computational materials engineering (ICME) links physics-based models to predict performance of materials based on their processing methods. Accurate models are essential in developing successful ICME. One such area of research is the recrystallization of beta-cogged titanium-aluminum alloys. Upon heat treatment, these materials undergo recrystallization, forming new grains with a low dislocation density. The phase field method is a kinetics- and thermodynamics-based model that simulates microstructural evolution. A polycrystalline microstructure is modeled with a separate order parameter for each grain; these order parameters are evolved according to Allen-Cahn dynamics. The recrystallization phase field model incorporates stored energy contributions and the nucleation of new undeformed grains. Stored energy due to dislocations is an additional driving force for microstructural evolution. An interpolation scheme has been developed to describe the stored energy across grain boundaries. Furthermore, the criteria for seeding newly recrystallized grains have been devised for a nucleation algorithm. The model has been parameterized for the titanium-aluminum system, and microstructural evolution is simulated for the binary alloy. The computationally obtained microstructures are compared with experimental recrystallization studies that were performed by collaborators. The recrystallized volume fraction and average grain size are measured as a function of alloy composition and annealing time. These microstructures are used as inputs for another ICME model that employs reduced order descriptors to efficiently account for microstructures in mechanical behavior simulations.

3:20 PM Break

3:40 PM

ICME Training in Materials Science and Engineering Curriculum: *Lan Li*[1]; [1]Boise State University

In tomorrow's materials science and engineering workplace, ICME modeling tools will be integral to optimize outcomes. Universities, national labs and industry already integrate such tools, with increasing use across scientific and engineering disciplines. However, undergraduate and graduate students new to the ICME methods can find them unrelated to their education and training. Teaching ICME is challenging because of limited time in a semester and complicated ICME topics. This year, the Department of Materials Science and Engineering at Boise State University redesigns its traditional computational materials science course, offered to senior undergraduate and graduate students, to gear towards the ICME topics. The course covers ICME overview, density functional theory, molecular dynamics, phase field simulations, and finite element analysis. In order to facilitate students' learning, we involve various activities, such as concept maps, group studies, ICME paper review, in-class practice, and instruction videos. We also apply a series of assessment tools to measure students' learning outcomes, such as in-class quizzes, students' presentations, ICME project proposal writing etc. This presentation will demonstrate the course outcomes and discuss the challenges of teaching ICME.

4:00 PM

Micro-bending Fatigue Testing of Ni and Ni-base Superalloys: Experiments Supporting ICME: *Zafir Alam*[1]; Jessica Krogstad[2]; David Eastman[1]; Thomas Straub[3]; Christoph Eberl[3]; Kevin Hemker[1]; [1]Johns Hopkins University; [2]University of Illinois; [3]Fraunhofer Institute for Mechanics of Materials

Development of physics-based life prediction models for fatigue is a challenging but important thrust area within the ICME paradigm. Insights on how local microstructure (grain size, shape, orientations and neighbourhoods) influence local plasticity and subsequent crack formation, derived from experiments at salient length scales, are vital for the development and benchmarking of the ICME-life prediction models. In this study, we present a novel ultrasonic resonance-based micro-bending fatigue setup and demonstrate its usefulness in ascertaining the effect of microstructure on the initiation of fatigue failure in ~500µm thick Ni and Ni-base superalloy foils. Fatigue damage is tracked by changes in resonance frequency and concomitant microstructure analyses. This allows for the direct experimental measurements of the number of cycles and microstructural locations associated with: slip initiation, persistent slip band formation, crack initiation, and intergranular

crack propagation. The local neighborhoods in which these critical events occurred have been characterized with orientation mapping, confocal microscopy and conventional imaging, and these experimental observations and results are being used as benchmarks for parallel multi-scale modeling and simulation efforts. The research is supported by the AFOSR and AFRL supported Center of Excellence on Integrated Materials Modelling (CEIMM).

4:20 PM

Expanding Dynamic Data Evaluation to Metals and Alloys: *Boris Wilthan*[1]; Vladimir Diky[1]; Erik Pfeif[1]; [1]NIST

The Thermodynamics Research Center (TRC) within NIST is actively engaged in developing standards and tools for the representation and interoperability of materials data from original literature and experiments. The approach adopted by TRC is dynamic data evaluation, whereby a reliable underlying data archive is used in conjunction with an algorithmically-encoded expert analysis in order to generate up-to-date data recommendations. The traditional focus of TRC's development of techniques, standards and tools has been material properties of small molecular organic compounds. Beginning in 2013, TRC began expanding its focus to include metals and alloys in support of the Materials Genome Initiative, a multi-agency effort designed to create a new era of policy, resources, and infrastructure that support U.S. institutions in the effort to discover, manufacture, and deploy advanced materials twice as fast, at a fraction of the cost. While the challenges in implementing such a system are significant, the potential benefits are undoubted. In stage one, data capture software has to be adapted to handle data for thermophysical properties of pure metals as well as the structures that come with experimental data from multiphase alloys. The presentation covers the overall methodologies required to efficiently and effectively convert information from published data into structured well-vetted datasets that can be then used as inputs for very large scale efforts in modeling, property-based literature searches or improving the quality of published information and preventing the propagation of erroneous data.

4:40 PM

Investigating Stress - Strain Partitioning in Nanostructured Multi-phase Alloys by Coupled Experiments and Simulations: *C. Cem Tasan*[1]; Dingshun Yan[1]; Martin Diehl[1]; Noriki Fujita[1]; Franz Roters[1]; Dierk Raabe[1]; [1]Max-Planck Institute for Iron Research

The mechanical response of multi-phase alloys is governed by the microscopic strain and stress partitioning behavior among microstructural constituents. Yet, due to limitations in the characterization of the partitioning that takes place at the sub-micron scale, microstructure optimization of such alloys is typically based on evaluating the averaged response, referring to e.g. macroscopic stress-strain curves. Here, a novel experimental–numerical methodology is introduced to strengthen the integrated understanding of microstructure and mechanical properties, enabling joint analyses of deformation-induced evolution of the microstructure, and the strain and stress distribution therein, down to sub-micron resolution. The capabilities of this approach is demonstrated through case studies on martensite–ferrite and bainite–martensite–austenite microstructures; and deviations are discussed in terms of limitations of techniques involved. Overall, the presented integrated computational materials engineering (ICME) approach provides vast amount of well-correlated structural and mechanical data that enhance our understanding and design capabilities of multi-phase alloys.

Plenary Session IV

Thursday AM
June 4, 2015

Room: Colorado II & III
Location: Cheyenne Mountain Resort

8:00 AM Invited

Modeling Across Length Scales: A Roadmapping Study: Peter Voorhees[1]; *George Spanos*; [1]Northwestern University

The emergence of Integrated Computational Materials Engineering (ICME) and the Materials Genome Initiative (MGI) as potential "game changers" for greatly reducing the time and cost of the discovery, development, and deployment of advanced materials and manufacturing processes has helped to highlight the great value of robust and accurate predictive simulations of materials behavior. A crucial element needed for implementing these predictive models and simulations into materials design and development is their integration across the product development cycle. This integration translates to a fundamental need for proper linkage of models across length (and time) scales. A significant shortcoming though with most existing computational tools is their inability to span the wide range of length and time scales that are of relevance to materials design. In this regard, The Minerals, Metals & Materials Society (TMS) has led a roadmapping study on this topic on behalf of the Material Measurement Laboratory of the U.S. National Institute of Standards and Technology (NIST). This study identifies gaps in our ability to bridge theses scales, and ascertains approaches and makes recommendations for critical steps and pathways for efficient, accurate, and automated integration of materials models and simulation codes used at various length and time scales. This presentation will provide an overview and some key highlights from that roadmapping study.

8:30 AM Invited

NIST and Materials Genome Initiative: *James Warren*[1]; [1]NIST

Over the past three years, NIST has invested considerable effort towards delivering infrastructure in support of the Administration's Materials Genome Initiative. To foster widespread adoption of the MGI Paradigm both across and within the multitude of materials development ecosystems, NIST is developing materials data and model exchange protocols and methods, the means to ensure the quality materials data and models and new methods and metrics for accelerated materials development. In this talk I will detail our successes and challenges in delivering on these broad mission elements and discuss opportunities for further progress.

8:50 AM Invited

ICME-Related Opportunities at the National Science Foundation: *Alexis Lewis*[1]; [1]National Science Foundation

Funding opportunities for work related to Integrated Computational Materials Engineering at the National Science Foundation will be discussed, with an emphasis on those opportunities in the Engineering directorate. The role of ICME in the Designing Materials to Revolutionize and Engineer our Future (DMREF) program will be presented, highlighting specific review criteria related to the integration of computational and/or theoretical work with experimental research in an iterative feedback loop. The requirements and expectations for the storage, sharing, and management of materials data will be presented in the context of the DMREF program. Other ICME-related funding opportunities will be presented, as well as general budget trends and focus areas throughout NSF.

9:10 AM Break

9:20 AM Invited
Rectifying Bottom-up and Top-down Uncertainties in Multiscale Modeling: *David McDowell*[1]; [1]Georgia Institute of Technology

We consider structure-property relations controlled by defects in crystal and polycrystals. Challenges of verification and validation of models at various scales of length and time are discussed. At a given scale of material structure hierarchy, dual routes of decision support exist via (i) consistency with mesoscale and macroscale experiments and (ii) results of bottom-up cascade of information obtained from lower scale, high fidelity models. Model form and model parameter uncertainty of both reducible (epistemic) and irreducible (aleatory) types are considered, and examples are given based on our work in modeling fatigue crack formation and early propagation processes in polycrystals, as well as using atomistics and higher scale experiments to inform mesoscale models such as material yield strength and rate dependence as a function of crystal orientation under nanoindentation, and the form of the kinetics relation (flow role) for migration of screw dislocations in bcc Fe. The issue of how a given model at the mesoscale can accept information from both bottom-up and top-down pathways is considered.

9:50 AM Invited
Microstructure Modelling in ICME Settings: *Georg Schmitz*[1]; Markus Apel[1]; Bernd Böttger[1]; [1]Access RWTH Aachen

The importance of microstructure simulations in ICME settings will be discussed with respect to their added value provided to macroscopic process simulations and their contribution to the prediction of materials properties. Their role in integrating the scales from component/process scale down to atomistic scales and also in integrating the experimental and virtual worlds will be highlighted. Practical implications for coupling a heterogeneous variety of codes and tools to microstructure simulations will be discussed using the example of the commercial multi-phase-field software MICRESS®. The presentation will conclude with some conceptual thoughts about a future standard format for the description of digital microstructures.

10:10 AM Break

10:30 AM Panel Discussion

11:30 AM Concluding Comments

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NOTES

CHEYENNE MOUNTAIN RESORT
colorado springs

Conference Level


LIFTED BY PHYSICS,
POWERED BY DREAMS.
The pioneers of aviation taught us that whatever the endeavor, passion and vision are the true drivers of innovation and success. Boeing is proud to salute those with the passion and vision to turn dreams into reality.
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