TMS ICME

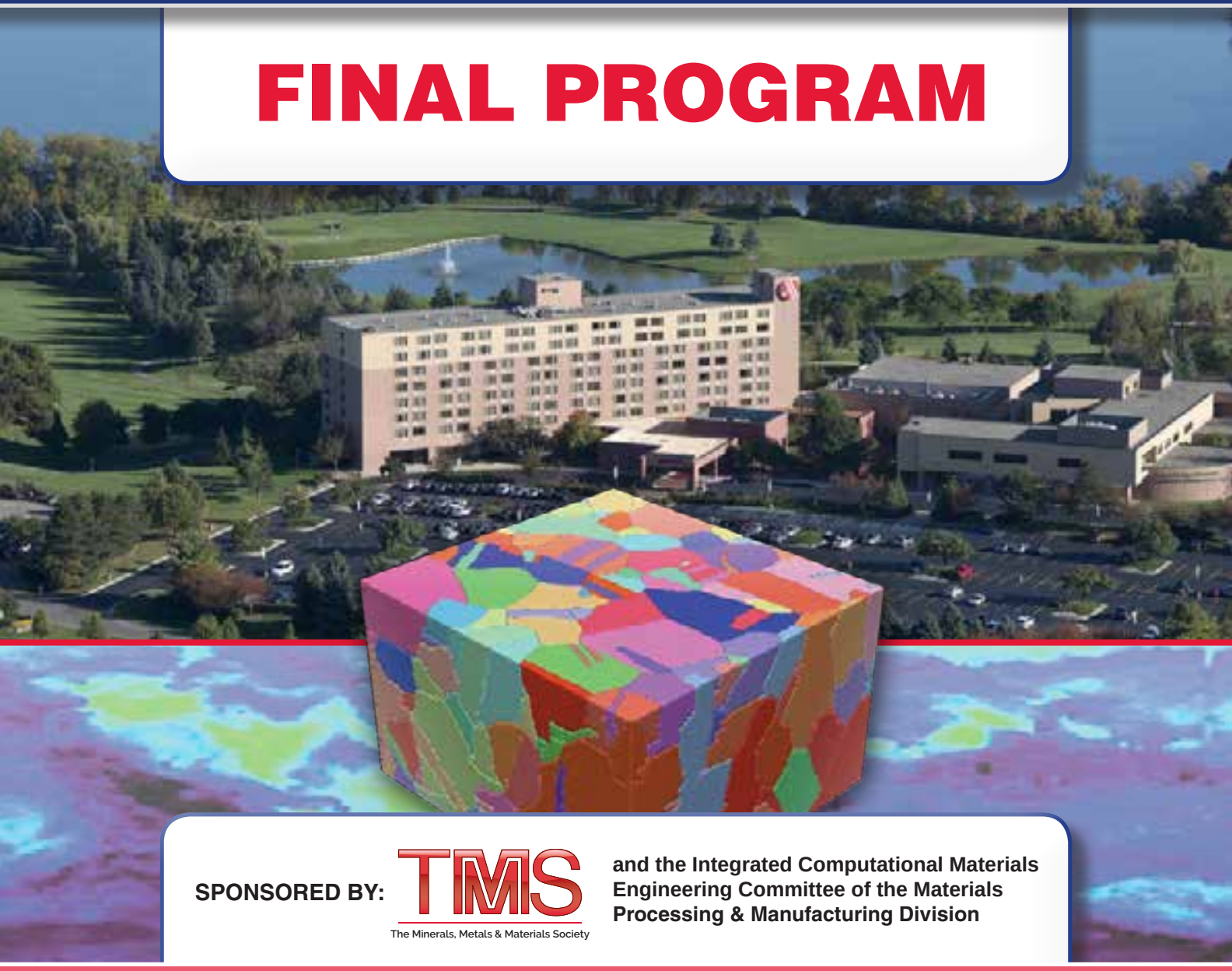
MANUFACTURING

DESIGN MATERIALS

4th World Congress on Integrated Computational Materials Engineering (ICME 2017)

May 21–25, 2017 • Marriott Ann Arbor Ypsilanti at Eagle Crest • Ypsilanti, Michigan, USA

FINAL PROGRAM



SPONSORED BY: TMS The Minerals, Metals & Materials Society and the Integrated Computational Materials Engineering Committee of the Materials Processing & Manufacturing Division

www.tms.org/ICME2017

SCHEDULE OF EVENTS

Technical Sessions held on Conference Center 1st Level - Salon I; Salons II and III; and Salon IV

Sunday, May 21

Registration	5:30 p.m. to 7:30 p.m.	Salon Ballroom Foyer
Welcome Reception	6:30 p.m. to 7:30 p.m.	Atrium

Monday, May 22

Registration	7:30 a.m. to 6:30 p.m.	Salon Ballroom Foyer
Plenary Session I	8:00 a.m. to 10:00 a.m.	Salon II, III, IV
Exhibition Set-up	8:00 a.m. to 10:00 a.m.	Salon V, VI
Break	10:00 a.m. to 10:30 a.m.	Salon Ballroom Foyer
Technical Sessions	10:30 a.m. to 12:10 p.m.	Conference Center 1st Level
Lunch	12:10 p.m. to 2:00 p.m.	On Your Own
Technical Sessions	2:00 p.m. to 3:30 p.m.	Conference Center 1st Level
Break	3:30 p.m. to 3:50 p.m.	Salon V, VI
Exhibition	3:30 p.m. to 6:30 p.m.	Salon V, VI
Technical Sessions	3:50 p.m. to 5:00 p.m.	Conference Center 1st Level
Poster Viewing and Reception	5:00 p.m. to 6:30 p.m.	Salon V, VI

Tuesday, May 23

Registration	7:30 a.m. to 6:00 p.m.	Salon Ballroom Foyer
Technical Sessions	8:00 a.m. to 10:00 a.m.	Conference Center 1st Level
Exhibition	10:00 a.m. to 5:50 p.m.	Salon V, VI
Break	10:00 a.m. to 10:30 a.m.	Salon V, VI
Technical Sessions	10:30 a.m. to 12:10 p.m.	Conference Center 1st Level
Lunch	12:10 p.m. to 2:00 p.m.	On Your Own
Plenary Session II	2:00 p.m. to 4:00 p.m.	Salon II, III, IV
Break	4:00 p.m. to 4:20 p.m.	Salon V, VI
Vendor Showcase	4:20 p.m. to 5:50 p.m.	Salon II, III, IV

Wednesday, May 24

Registration	7:30 a.m. to 5:00 p.m.	Salon Ballroom Foyer
Plenary Session III	8:00 a.m. to 10:00 a.m.	Salon II, III, IV
Exhibition	10:00 a.m. to 3:50 p.m.	Salon V, VI
Break	10:00 a.m. to 10:30 a.m.	Salon V, VI
Technical Sessions	10:30 a.m. to 12:30 p.m.	Conference Center 1st Level
Lunch	12:30 p.m. to 2:00 p.m.	On Your Own
Technical Sessions	2:00 p.m. to 3:30 p.m.	Conference Center 1st Level
Break	3:30 p.m. to 3:50 p.m.	Salon V, VI
Technical Sessions	3:50 p.m. to 5:00 p.m.	Conference Center 1st Level
Exhibition Dismantle	After 3:50 p.m.	Salon V, VI
Congress Dinner	6:00 p.m. to 8:00 p.m.	Garden Marquee

Thursday, May 25

Registration	7:30 a.m. to Noon	Salon Ballroom Foyer
Technical Sessions	8:00 a.m. to 10:00 a.m.	Conference Center 1st Level
Break	10:00 a.m. to 10:20 a.m.	Salon Ballroom Foyer
Plenary Session IV	10:20 a.m. to 11:40 a.m.	Salon II, III, IV
Closing Remarks	11:40 a.m. to Noon	Salon II, III, IV
PRedictive Integrated Structural Materials Science (PRISMS) Workshop*	Noon to 5:00 p.m.	PRISMS Center, University of Michigan

Friday, May 26

PRedictive Integrated Structural Materials Science (PRISMS) Workshop*	8:00 a.m. to 5:00 p.m.	PRISMS Center, University of Michigan

** This workshop required separate registration.*

TABLE OF CONTENTS

WELCOME TO THE 4TH WORLD CONGRESS ON INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING!

On behalf of The Minerals, Metals & Materials Society (TMS) and the congress organizing committee, we are pleased to welcome you to the 4th World Congress on Integrated Computational Materials Engineering (ICME 2017). The materials science and engineering field is at a critical juncture in its evolution, in large part due to our community's bold vision for the future of materials discovery, design, development, manufacture, and deployment through the Materials Genome Initiative (MGI) and integrated computational materials engineering (ICME). Building on the great success of the first three world congresses on ICME in 2011, 2013, and 2015, ICME 2017 will convene stakeholders—including researchers, educators, and engineers—to discuss the recent global advancement of ICME as an engineering discipline. As we approach the close of the first decade since 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 2017.

Warmest regards on behalf of the Organizing Committee.

PRedictive Integrated Structural Materials Science (PRISMS) Workshop

Thursday, May 25–Friday, May 26 • University of Michigan • Ann Arbor, Michigan, USA

This workshop will provide attendees with an in-depth understanding of and the ability to use the PRISMS Software Tools. Stop by the registration desk (located in the Salon Ballroom Foyer) to register for the workshop and enhance your congress experience.

The workshop will be held at the PRISMS Center on the University of Michigan campus, located about 10 miles from the Ann Arbor Marriott Ypsilanti at Eagle Crest (the ICME 2017 congress location). For attendees staying at the Marriott, bus transportation to and from the PRISMS Center will be provided. Bus departure times are:

	Depart Ann Arbor Marriott Ypsilanti at Eagle Crest to PRISMS Center	Depart PRISMS Center to Ann Arbor Marriott Ypsilanti at Eagle Crest
Thursday, May 25	Noon	5:00 p.m.
Friday, May 26	8:00 a.m.	5:00 p.m.

The workshop registration fee ($150) includes 1.5 days of instruction, refreshment breaks, lunch on both workshop days, course materials, and transportation between the hotel and workshop location.

The PRISMS Workshop is hosted by the PRISMS Center at the University of Michigan.

ABOUT THE CONGRESS

ORGANIZING COMMITTEE

CHAIR:
- Paul Mason, Thermo-Calc Software, USA

CO-CHAIRS:
- Charles R. Fisher, Naval Surface Warfare Center - Carderock Division, USA
- Ryan Glamm, The Boeing Company, USA
  Michele V. Manuel, University of Florida, USA
- Georg J. Schmitz, MICRESS group at ACCESS e.V., Germany
- Amarendra K. Singh, Indian Institute of Technology, Kanpur, India
- Alejandro Strachan, Purdue University, USA

INTERNATIONAL ADVISORY COMMITTEE:
- Dipankar Banerjee, Indian Institute of Technology, India
- Annika Borgenstam, KTH – Royal Institute of Technology, Sweden
- Masahiko Demura, National Institute for Materials Science, Japan
- Dennis Dimiduk, BlueQuartz, LLC, USA
- B.P. Gautham, Tata Consulting Services, India
- Liang Jiang, Central South University, China
- Kai-Friedrich Karhausen, Hydroaluminium, Germany
- Peter Lee, Imperial College, UK
- Mei Li, Ford Motor Company, USA
- Baicheng Liu, Tsinghua University, China
- Javier Llorca, IMDEA, Spain
- Jiangfeng Nie, Monash University, Australia
- Warren Poole, University of British Columbia, Canada
- Antonio J. Ramirez, The Ohio State University, USA
- James Warren, National Institute of Standards and Technology, USA
- Erich Wimmer, Materials Design, France

REGISTRATION

Your registration badge ensures admission to each of these events:

- Technical and Poster Sessions
- Sunday Welcome Reception
- Monday Networking Reception
- Wednesday Congress Dinner*

** Please note that while one ticket for the congress dinner is included, registration was required for this event through the congress registration form. Check at the registration desk (Salon Ballroom Foyer) for more information.*

REGISTRATION HOURS
The registration desk will be located in the Salon Ballroom Foyer.

Sunday	5:30 p.m. to 7:30 p.m.
Monday	7:30 a.m. to 6:30 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 Noon

CONGRESS DETAILS

INTERNET ACCESS
Complimentary wireless internet access is available in the conference areas of the Marriott Ann Arbor Ypsilanti at Eagle Crest hotel. The wireless network is named “ICME2017” and the password is “ICME2017.” Complimentary high speed internet is available in all guest rooms.

TECHNICAL SESSIONS
All oral presentations will be held on the 1st level of the Conference Center in Salons I through IV. All poster presentations will be held in Salon V and VI. See the Technical Program section on pages 18-45 for room locations.

PROCEEDINGS
Full congress registrants will receive one hard copy of the proceedings publication and electronic access to the same content as part of the registration fee. Complimentary proceedings content **must be downloaded before June 30, 2017,** at which time standard pricing will take effect. Additional hard copies and e-books may be purchased at www.springer.com (TMS members receive a 20% discount).

EXHIBITION

EXHIBITION HOURS
The exhibition will be located on the 1st level of the Convention Center in Salons V and VI.

Monday, May 22
Set-Up: 8:00 a.m. to 10:00 a.m.
Exhibit Hours: 3:30 p.m. to 6:30p.m.

Tuesday, May 23
Exhibit Hours: 10:00 a.m. to 5:50 p.m.
Break: 10:00 a.m. to 10:30 a.m. and 4:00 p.m. to 4:20 p.m.
Vendor Showcase: 4:20 p.m. to 5:50 p.m.

Wednesday, May 24
Exhibit Hours: 10:00 a.m. to 3:50 p.m.
Break: 10:00 a.m. to 10:30 a.m. and 3:30 p.m. to 3:50 p.m.
Exhibit Dismantle: After 3:50 p.m.

WELCOME TO TMS

The Minerals, Metals & Materials Society

DID YOU KNOW?

If you registered for ICME 2017 at the nonmember rate, your registration includes a TMS electronic membership through the end of the year.

WHAT CAN YOU DO WITH YOUR NEW MEMBERSHIP?

- **Read:** Access more than 20 journals published by TMS and Springer for free and explore online publication libraries available only to members
- **Network:** Join a TMS technical committee or connect with colleagues through the TMS Membership Directory
- **Advance Your Career:** Post your resume on the TMS Career Center or download the PE Exam Study Guide for Metallurgical and Materials Engineering
- **And Much More!**

Visit **members.tms.org** to view a complete listing of benefits available to you as a TMS member.

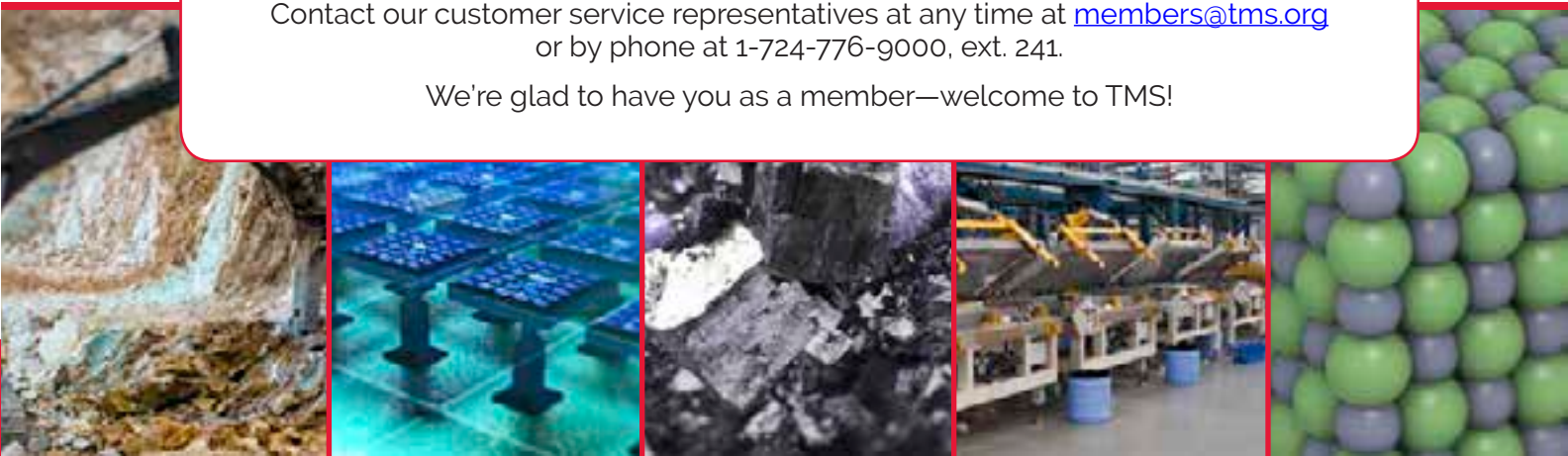
HOW CAN YOU ACCESS YOUR BENEFITS?

Following the meeting, you'll receive an e-mail from TMS with your member username and password. Once you receive this, you can log in to the "Access Member Benefits" section of the TMS website at members.tms.org.

QUESTIONS?

Contact our customer service representatives at any time at members@tms.org or by phone at 1-724-776-9000, ext. 241.

We're glad to have you as a member—welcome to TMS!



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

PLATINUM SPONSORS

U.S. DEPARTMENT OF ENERGY

Department of Energy,
Advanced Manufacturing Office

The Office of Energy Efficiency and Renewable Energy's (EERE) Advanced Manufacturing Office (AMO) within the U.S. Department of Energy, brings together manufacturers, not-for-profit entities, institutes of higher education, national laboratories, and state and local governments to develop and deploy cutting-edge manufacturing technologies. These technologies are critical to a more efficient and competitive U.S. manufacturing sector, for the competitive domestic manufacture of clean energy products, to efficiently use abundant and low-cost energy resources in manufacturing, and to support improved energy productivity across the entire U.S. economy.

Ford

ONE FORD

ONE TEAM • ONE PLAN • ONE GOAL

Ford Motor Company

GOLD SPONSOR

TATA CONSULTANCY SERVICES

Tata Consulting

Tata Consultancy Services is an IT services, consulting and business solutions organization that delivers real results to global business, ensuring a level of certainty no other firm can match. TCS offers a consulting-led, integrated portfolio of IT, BPS,infrastructure, engineering and assurance services. This is delivered through its unique Global Network Delivery Model™, recognized as the benchmark of excellence in software development. TCS has a strong Research and Innovation unit, a network of Innovation Labs worldwide as well a Co-innovation Network that connects to Academic Alliances, Emerging Technology Ecosystems, Group companies and Anchor Customers. TCS research in process engineering has been active for more than thirty years. A part of the Tata group, India's largest industrial conglomerate, TCS has over 378,000 of the world's best-trained consultants in 45 countries. The company generated consolidated revenues of US $16.5 billion for year ended March 31, 2016 and is listed on the BSE (formerly Bombay Stock Exchange) and the NSE (National Stock Exchange) in India. For more information, visit us at www.tcs.com.

SILVER SPONSOR

WIAM unfreezing material knowledge

WIAM GmbH

For more than 45 years, IMA Dresden and WIAM have been supporting companies in efficiently and flexibly establishing and managing data. With WIAM software solutions, companies comply with national and international standards and guidelines regarding traceability and the legal obligation to preserve documents and data. WIAM offers information systems to support companies with (material) data management. Easy search, filter and comparison functionalities help people to find, manage and link data while making it available to other applications such as ERP, PDM and CAE. Moreover, IMA Dresden develops and tests materials, parts, products for the automotive, aircraft, railway and medical industries.

BRONZE SPONSORS

Thermo-Calc Software

A leading developer of software and databases for calculations involving computational thermodynamics and diffusion controlled simulations. Thermo-Calc: a powerful tool for thermodynamic calculations for multicomponent systems. DICTRA: a module for accurate prediction of diffusion in multicomponent alloys. TC-PRISMA: a module for simulations of precipitation kinetics. Thermodynamic and kinetic databases are developed using the CALPHAD approach and more than forty databases are available for steels, Ti, Al-, Mg-, HEAs, Ni-superalloys and other materials. From 2017 a new Property Model Development Framework has been introduced to allow users to develop their own property models written in Python and integrate them into Thermo-Calc.

QuesTek Innovations

As a global leader in Integrated Computational Materials Engineering (ICME) technologies, QuesTek Innovations LLC is at the forefront of designing new materials and accelerating their implementation into demanding applications. QuesTek has applied its ICME-based technology and its *Materials by Design*® methodology to successfully design four advanced steels that are commercially available through Carpenter Technology and utilized in aerospace applications. QuesTek provides solutions to demanding materials challenges in industry, ranging from power generation to oil & gas, by designing a wide array of alloys such as Ni-based alloys, stainless steels, high entropy alloys and alloys tailored specifically for additive manufacturing.

Pratt & Whitney

Pratt & Whitney develops game-changing technologies for the future. The company's worldwide large commercial engine maintenance, repair and overhaul network provides innovative services that add value and delight customers around the globe. Pratt & Whitney's large commercial engines power more than 25 percent of the world's mainline passenger fleet. The company continues to develop new engines and work with its partners in International Aero Engines and the Engine Alliance to meet airline customers' future needs.

MICRESS

MICRESS® - the MICRostructure Evolution Simulation Software – allows for the simulation of microstructure formation in metallurgical systems. It is developed, maintained and distributed by ACCESS e.V., a non-profit research centre at the RWTH Aachen University of Technology. The strength of MICRESS® is the comprehensive treatment of thermodynamic equilibria, diffusion and curvature. Commercial thermodynamic datasets allow to simulate microstructure evolution during solidification and solid state transformations in alloy systems of technical interest. MICRESS® especially allows for optimisation of processes and for the development of new alloys. MICRESS® is installed around the globe at various sites from industry, research centres and universities.

Thermo-Calc Software

Powerful Software for Thermodynamic and Diffusion Calculations

Changing the Paradigm for Materials Design

Through CALPHAD Based Software

Technology is moving materials design to a better paradigm, computational materials software.

- ✓ **Predict** what phases form as a function of composition and temperature
- ✓ **Reduce** costly, time-consuming experiments
- ✓ **Base decisions** on scientifically supported predictions and data
- ✓ **Shorten** development time and accelerate materials development while reducing risk
- ✓ **Improve** the quality and consistency of your products through deeper understanding of your materials and processes

Watch a webinar to learn about applications to ICME

www.thermocalc.com/webinars

Thermo-Calc Software AB
Email: info@thermocalc.com
Phone: +46-8-545 959 30

www.thermocalc.com

USA, Canada and Mexico
Email: paul@thermocalc.com
Phone: (724) 731 0074

National Institute of Standards and Technology (NIST)
NIST is working to build the materials innovation infrastructure in support of the Materials Genome Initiative. Our mission is to accelerate materials innovation with a material genome approach to decrease the cost and time-to-market by 50%. A variety of data repositories and registries, data curation tools, data integration tools, and modeling tools are being developed to support this materials innovation infrastructure.

EXHIBITORS

Math2Market
Math2Market GmbH is a German company that develops and markets the software GeoDict. We are a leader in providing software and consulting solutions for non-destructive testing and the design of innovative materials. Our scientific software GeoDict models materials using 3D-image data or user-defined parameters, and simulates their properties to reduce or eliminate expensive and time-consuming laboratory tests.

HPC for Manufacturing Program
The HPC for Manufacturing Program (HPC4Mfg) unites the world-class computing resources and expertise of Department of Energy national laboratories with the U.S. manufacturers to deliver solutions that could revolutionize manufacturing. Led by Lawrence Livermore National Laboratory (LLNL), and joined by its partners, Lawrence Berkeley and Oak Ridge national laboratories, HPC4Mfg offers a low-risk path for U.S. manufacturing companies interested in adopting high-performance computing (HPC) technology to advance clean energy technologies and increase energy efficiency while reducing risk of HPC adoption. The HPC4Mfg Program aims to infuse advance computing expertise and technology into the manufacturing industry; advance innovative clean energy technologies; reduce energy and resource consumption; and increase U.S. competitiveness. The HPC4Mfg Program conducts solicitations twice a year to select projects for collaboration. The Department of Energy's Advanced Manufacturing Office (AMO) within the Energy Efficiency and Renewable Energy (EERE) Office, sponsors this program.

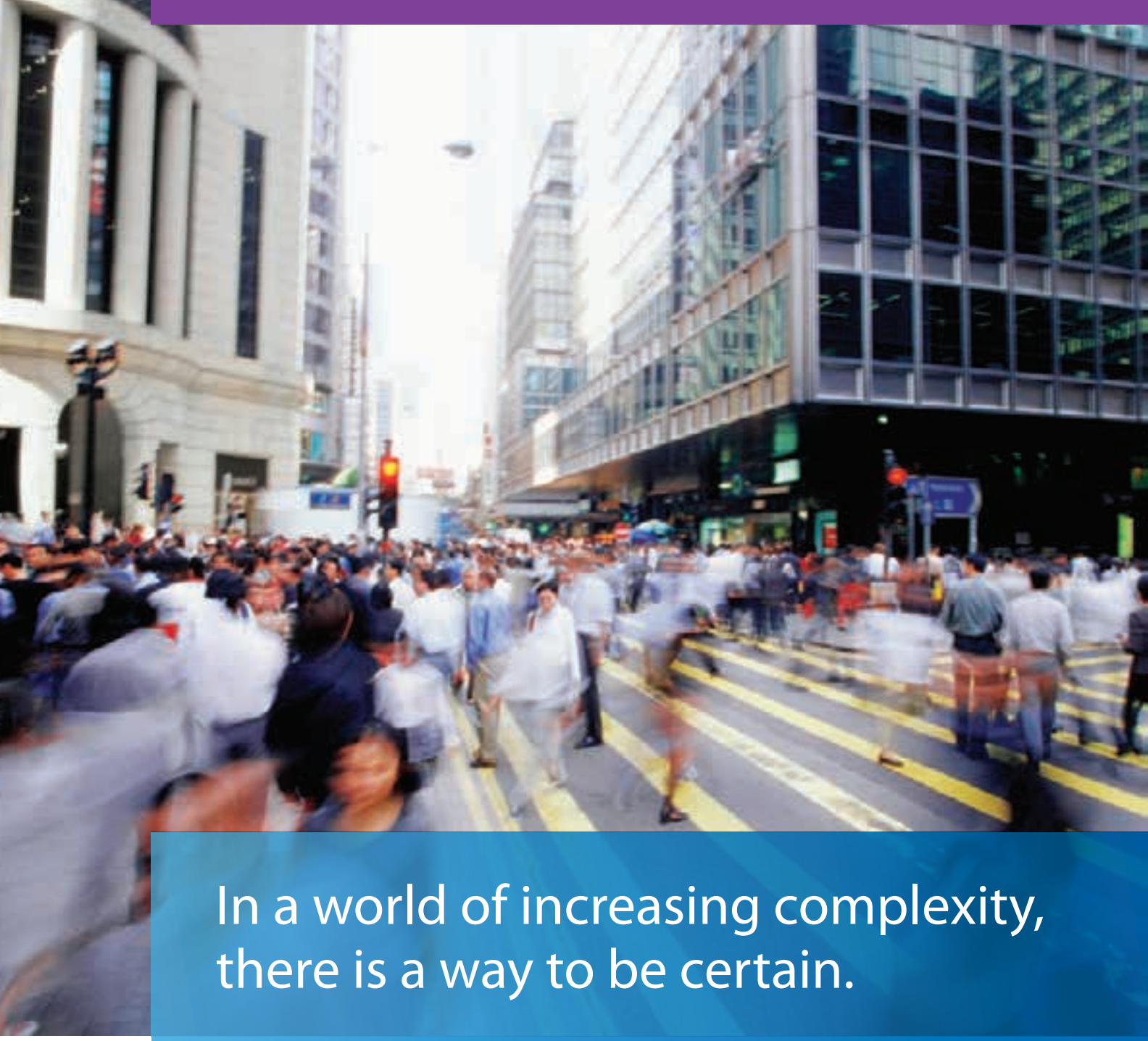
GOVERNMENT SUPPORT PROVIDED BY:

National Science Foundation (NSF)
As indicated on their website, the NSF "promotes the progress of science; to advance the national health, prosperity, and welfare; and to secure the national defense." The NSF's goals—discovery, learning, research infrastructure, and stewardship—provide an integrated strategy to advance the frontiers of knowledge, cultivate a world-class, broadly inclusive science and engineering workforce and expand the scientific literacy of all citizens, build the nation's research capability through investments in advanced instrumentation and facilities, and support excellence in science and engineering research and education through a capable and responsive organization.
www.nsf.gov

VENDOR SHOWCASE

Tuesday, May 23
Don't miss the Vendor Showcase! This event provides an opportunity for vendors and developers to meet and discuss new tools and techniques with congress attendees. Companies featured in the showcase include:

4:20 p.m.: National Institute of Standards and Technology (NIST)
4:30 p.m.: MICRESS
4:40 p.m.: QuesTek
4:50 p.m.: Math2Market
5:00 p.m.: Thermo-Calc Software
5:10 p.m.: Tata Consultancy Services
5:20 p.m.: WIAM GmbH



In a world of increasing complexity, there is a way to be certain.

Research Based Innovation in TCS enables its customers gain competitive advantage, in a fast changing world of technology

For more information on TCS Research and Innovation, email us at innovation.info@tcs.com or visit us at www.tcs.com/research

TATA

IT Services
Business Solutions
Consulting

TATA CONSULTANCY SERVICES
Experience certainty.

NETWORKING & SOCIAL EVENTS

WELCOME RECEPTION

The Welcome Reception will be held on Sunday, May 21, from 6:30 p.m. to 7:30 p.m. in the Atrium on the 1st level of the Conference Center.

POSTER VIEWING/NETWORKING RECEPTION

A Networking Reception is planned for Monday, May 22, from 5:00 p.m. to 6:30 p.m. in Salons V and VI. Don't miss this great networking opportunity!

CONGRESS DINNER

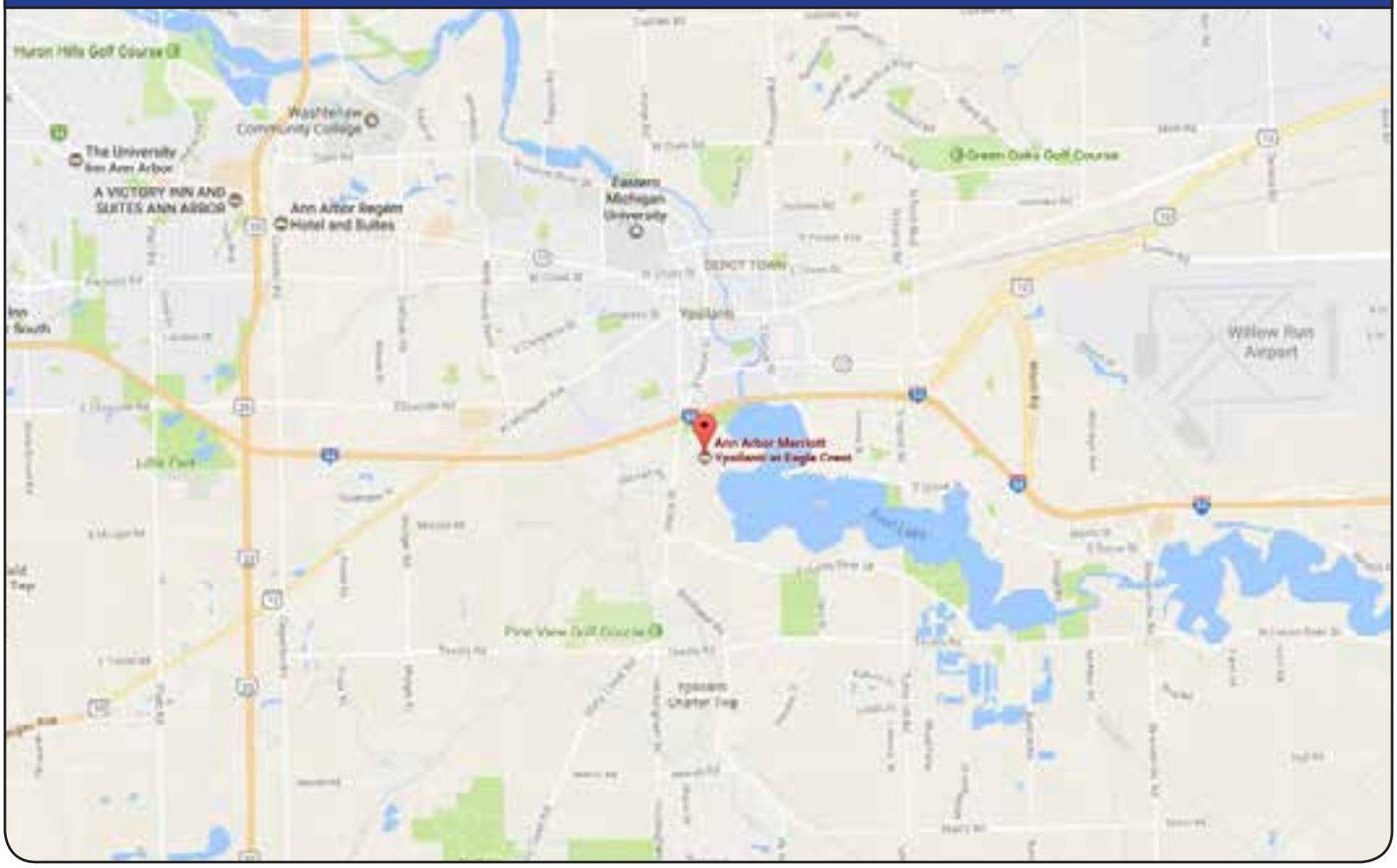
The dinner will be held on Wednesday, May 24, from 6:00 p.m. to 8:00 p.m. in the Garden Marquee.
Please note that while one ticket for the congress dinner is included, registration was required for this event through the congress registration form. Onsite ticket sales are based on availability. Check with TMS staff at the registration desk (Salon Ballroom Foyer) for more information.

ABOUT THE VENUE

The Ann Arbor Marriott Ypsilanti at Eagle Crest hotel is conveniently located 20 minutes from the Detroit Metro Airport (DTW) and 45 minutes from downtown Detroit. Situated on 135 acres, the Ann Arbor Marriott Ypsilanti at Eagle Crest hotel offers tranquil, resort-like accommodations. High speed internet in all guest rooms and complimentary onsite parking are just two of the hotel's many amenities. Visit the hotel website for more information on:

- A variety of local attractions and activities
- Dining options, both onsite at the hotel and located nearby

VENUE AREA MAP



PLENARY SPEAKERS

- "Integrated Computational Materials Engineering 2017," **Julie A. Christodoulou**, Office of Naval Research
- "TMS Materials Data Infrastructure Study," **Charles H. Ward**, Air Force Research Laboratory
- "Towards an ICME Methodology - Current Activities in Europe," **Georg J. Schmitz**, Micress/ Aachen
- "The Generalized CALPHAD Methodology – The Data Infrastructure of ICME," **John Agren**, Royal Institute of Technology
- "Innovations in Experimental Techniques for ICME," **Ji-Cheng Zhao**, The Ohio State University
- "Robust Information Management System Enabling Multiscale Modeling Within ICME Paradigm," **Steven M. Arnold**, NASA Glenn Research Center
- "ICME Guided Cast Aluminum and Steel Alloys Development in Automotive Applications," **Mei Li**, Ford Motor Company
- "Uncertainty Management and Decision Making in the ICME Process Chain," **Jitesh H. Panchal**, Purdue University
- "The Materials Project for Accelerated Design of Energy Materials," **Muratahan Aykol**, Lawrence Berkeley National Laboratory
- "European Materials Modelling Council," **Nadja Adamovic**, TU Wien
- "Workforce Development for Materials Science & Engineering of the Future," **Katsuyo Thornton**, University of Michigan

Integrating Materials and Manufacturing Innovation

The Technical Publishing Home for ICME Tools, Application, and Impact

Designed to the Needs of the ICME Community

Integrating Materials and Manufacturing Innovation (*IMMI*) offers a highly focused technical scope to address key topical areas that have been underserved by peer-reviewed journals in the past. *IMMI* specifically concentrates on four themes supporting integrated computational materials engineering (ICME):

Data | **Tools** | **Application** | **Impact**

Charles H. Ward
Editor-in-Chief

Distinguish Your Work

Rigorous peer review and an editorial board that counts some of the field's most esteemed leaders among its members ensures that your work will be highly regarded. *IMMI* has been selected for coverage in Thomson Reuters' Emerging Sources Citation Index (ESCI), beginning with 2016.

Publish Today

The *IMMI* publishing platform offers both protected and open access publishing options, with no mandatory fee for standard submissions.

Publishers:

TMS Springer

To submit your paper, visit https://www.editorialmanager.com/immj

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 April 21, 2017. 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.

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

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 U.S. and foreign antitrust laws and regulations.

TMS DIVERSITY AND INCLUSION STATEMENT

The Minerals, Metals & Materials Society (TMS) is committed to advancing diversity in the minerals, metals, and materials professions, and to promoting an inclusive professional culture that welcomes and engages all who seek to contribute to the field. TMS recognizes that a diverse minerals, metals, and materials workforce is critical to ensuring that all viewpoints, perspectives, and talents are brought to bear in addressing complex science and engineering challenges. To build and nurture this diverse professional community, TMS welcomes and actively engages the participation of underrepresented groups in all of its initiatives and endeavors.

EMERGENCY PROCEDURES

The chances of an emergency situation occurring at ICME 2017 are quite small. However, being prepared to react effectively in case of an incident is the most critical step in ensuring the health and safety of yourself and those around you. Please take a few moments to review the map of the Marriott Ann Arbor Ypsilanti at Eagle Crest facility printed in this program (on page 63). When you enter the building, familiarize yourself with the exits and the stairs leading to those exits. When you arrive at your session or event location, look for the emergency exits that are in closest proximity to you.

In case of a fire, please exit room and proceed outside onto the Conference Center Patio and out to the parking lot. Eagle Crest staff will provide instructions at this point.

In case of a tornado, please exit the room and proceed down the stairs to the lobby. Eagle Crest staff will direct attendees to safety in the basement of the hotel.

Please use the following local safety and security contact information if you or someone near you is experiencing an emergency:

Police Department: Michigan State Police
Telephone: 911 or 1-734-482-1211
Distance: 1/4 mile from hotel

Fire Department: Ypsilanti Township Fire Department
Telephone: 911 or 1-734-544-4244
Distance: Approx. 2 miles from hotel

Nearest Hospital: St. Joseph Mercy Hospital
Telephone: 1-734-712-3456
Distance: 5-6 miles from hotel

Alternate Hospital: University of Michigan Hospital
Telephone: 1-734-936-4000
Distance: 10-12 miles from hotel

SPURRING
INNOVATION, ECONOMIC GROWTH AND JOB CREATION
IN MANUFACTURING AND ENERGY

The **Advanced Manufacturing Office (AMO)**, within the U.S. Energy Department, is the only technology office within the U.S. Government that is dedicated to improving the energy and material efficiency, productivity, and competitiveness of manufacturers across the United States. We partner with industry, small business, universities, regional entities, and other stakeholders to identify and invest in emerging clean energy technologies. Through our technical partnerships with private sector partners, we can accelerate the eventual adoption by the private sector of new technologies and identify technical challenges faced by manufacturers that can be addressed through early-stage applied research and development. And by targeting efficient manufacturing technologies, AMO seeks to drive energy productivity improvements in the U.S. manufacturing sector, efficiently utilize abundant and available domestic energy resources, and support the manufacture of clean energy products with benefits extending across the economy.

The Advanced Manufacturing Office is a proud sponsor of the Integrated Computations Materials Engineering (IMCE).

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

ADVANCED MANUFACTURING OFFICE

U.S. Department of Energy Advanced Manufacturing Office
Room 5F-065, MS EE-5A | 1000 Independence Ave SW | Washington, DC 20585 | Phone: (202) 586-9488
WWW.MANUFACTURING.ENERGY.GOV

TECHNICAL PROGRAM GRID

Monday

All-Conference Joint Plenary

Salon I	Salon II, III	Salon IV
Plenary I Salon II, III, IV		
Break (30)		
Integration Framework and Usage IA	Additive Manufacturing I	Microstructure Evolution I
Lunch on Own (110)		
Integration Framework and Usage IB	Additive Manufacturing II	Microstructure Evolution II
Break (20)		
Integration Framework and Usage IB (continued)	Additive Manufacturing II (continued)	Microstructure Evolution II (continued)

Poster Session and Reception
Salon V, VI

Sunday: Welcome Reception
Thursday afternoon: PRISMS Workshop
Friday all day: PRISMS Workshop

Tuesday

Breakout Sessions

Salon I	Salon II, III	Salon IV
Mechanical Performance using Multi-Scale Modeling	Microstructure Evolution III	Phase Field Modeling I
Break (30)		
Mechanical Performance using Multi-Scale Modeling (continued)	Microstructure Evolution III (continued)	Phase Field Modeling I (continued)
Lunch on Own (110)		
All-Conference Joint* Session		
Plenary II Salon II, III, IV		
Break (20)		
Vendor Showcase - Software Solutions Salon II, III, IV		

Wednesday

All-Conference

Salon I	Salon II, III	Salon IV
Plenary III Salon II, III, IV		
Break (30)		
ICME Design Tools and Application I	Integration Framework and Usage IIA	ICME Success Stories and Applications I
Lunch on Own (90)		
Breakout Sessions		
ICME Design Tools and Application II	Integration Framework and Usage IIB	ICME Success Stories and Applications II
Break (20)		
ICME Design Tools and Application II (continued)	Integration Framework and Usage IIB (continued)	ICME Success Stories and Applications II (continued)

Congress Dinner
Garden Marquee

Thursday

All-conference

Salon I	Salon II, III	Salon IV
Verification, Validation, Uncertainty Quantification Issues and Gap Analysis	Phase Field Modeling II	ICME Success Stories and Applications III
Break (20)		
Plenary IV Salon II, III, IV		
Closing Remarks		

Share the Knowledge
Encourage Your Colleagues to Download the New TMS Report on *Building a Materials Data Infrastructure*

www.tms.org/MDIstudy

As part of your ICME2017 registration, you have already received a hard copy of this new report led by TMS on behalf of the U.S. National Science Foundation. Be sure to visit www.tms.org/MDIstudy to download a free copy to your computer and mobile device—and tell your colleagues to do the same.

Plenary I

Monday AM
May 22, 2017

Room: Salon II, III, IV
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

8:00 AM Invited
Integrated Computational Materials Engineering, 2017: *Julie Christodoulou*[1]; [1]Office of Naval Research

Nearly ten years has passed since the discipline of Integrated Computational Materials Engineering (ICME) was defined in the National Academies Report of 2008, and we find ourselves in the fourth World Congress on ICME. In this talk we'll re-evaluate some of the early observations and motivations leading to the ICME study, assess our progress toward very ambitious goals, celebrate a little, identify persistent challenges, and begin to scope what lays ahead.

8:40 AM Invited
TMS Materials Data Infrastructure Study: *Charles Ward*[1]; [1]Air Force Research Laboratory

The Minerals, Metals and Materials Society, with sponsorship from the National Science Foundation, conducted a study to define the actions needed to support the creation of a materials data infrastructure. Such an infrastructure is key to retaining, discovering, sharing, and reusing the digital materials data needed to power the discipline of Integrated Computational Materials Engineering and achieve the goals of the Materials Genome Initiative. Access to relevant materials data is becoming ever more important to the conduct of science and engineering throughout the lifecycle of a material, encompassing material discovery, development, product design, manufacturing and sustainment. A core team of experts was convened over the course of 14 months to explore the hurdles and opportunities involved with storing and sharing materials data including standards, supportability, sustainability, integration with publications, training and education, incentives and disincentives. Using content captured from their meetings along with input from supplemental interviews and workshops, the team developed a report with recommendations of key steps and pathways needed to realize a vision for a materials data infrastructure.

9:20 AM Invited
Towards an ICME Methodology- Current Activities in Europe: *Georg J. Schmitz*[1]; [1]Micress/Aachen

Scope of this presentation is to provide an overview about activities towards an ICME methodology currently going on in Europe. The presentation will especially introduce the European Materials Modelling Council (EMMC) as a bottom-up activity of the European materials modelling community and provide a short outline of the different working groups within the EMMC and their objectives. A short introduction of the ICMEg Coordination and Support Action and the lessons learned during its 3 years of activities will highlight the vision of plug& play in future ICME and emphasize the needs for interoperability and standardization as strategy to reach interoperability. Technical aspects of ICME like the development of simulation platforms, metadata descriptors and creating metadata schemata, which are elaborated within five different European research projects (MoDeNa, Deepen, Simphony, MMP and NanoSim), conclude the presentation. The research leading to these results has been performed within the ICMEg project and has received funding from the European Union Seventh Framework Programme (FP7/2007-2011] under grant agreement n° 6067114

10:00 AM Break

Integration Framework and Usage - IA

Monday AM
May 22, 2017

Room: Salon I
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

10:30 AM
A Vision for Mutliscale Materials and Structural Modeling: *David Furrer*[1]; Xuan Liu[1]; [1]Pratt & Whitney

Materials modeling has been rapidly advancing to enable significant changes in how materials area design, developed, defined and implemented. Computational tools and methods are becoming commonplace for many applications. As the materials engineering is evolving, there has also been a progressive acceptance of computational materials engineering into other engineering disciplines, such as design and structural engineering. The future of integrated multiscale materials engineering with other disciplines has been assessed and a vision for this future-state has been constructed. Based on this future-state target, a detailed review of the current technology gaps has been assembled. This effort has provided clear actions that must be taken on by the community to achieve this envisioned future state of multiscale materials and structural engineering. A summary of this effort and proposed actions will be provided.

10:50 AM
Insertion of ICME Paradigm to Shipbuilding through Process Simulation: *Charles Fisher*[1]; [1]Naval Surface Warfare Center

The integrated computational materials engineering (ICME) paradigm has found increased use across the scientific community to enable reduction of costly physical testing and improve efficiency in design selection. Within shipbuilding, the use of computational simulations is prevalent for structural finite-element analysis. However, current practice for FEA simulations does not integrate material processing into the structural design or failure-mode prediction calculations. Thus, the influence of residual stress and distortion induced by the fabrication process are not included in the simulation, yielding uncertainty in the computational models. To address this, numerous projects have initiated to validate thermal loading conditions and computational weld mechanics (CWM) techniques. Programs involving crack mitigation through residual stress reduction at welded joints, physical validation of CWM techniques, and computational software integration will be discussed, as well as identification of technical gaps for implementation. The end goal is improved confidence in, and use of, ICME techniques in order to better serve the shipbuilding enterprise.

11:10 AM
An Attempt to Integrate Software Tools at Microscale and Above Towards an ICME Approach for Heat Treatment of a DP Steel Gear with Reduced Distortion: *Deepu John*[1]; Hamidreza Farivar[2]; Gerald Rothenbucher[3]; Ranjeet Kumar[3]; Pramod Zagade[4]; Danish Khan[4]; Aravind Babu[1]; BP Gautham[4]; Ralph Bernhardt[3]; G. Phanikumar[1]; Ulrich Prahl[2]; [1]Indian Institute of Technology Madras; [2]Institut für Eisenhüttenkunde(IEHK); [3]Simufact Engineering GmbH; [4]TRDDC, TCS Research, Tata Consultancy Services

Finite element simulation of heat treatment cycles in steel could be challenging when it involves phase transformation at the microscale. An ICME approach that can take into account the microstructure changes during the heat treatment and the corresponding changes in the macroscale properties could greatly help these simulations. Inter-critical annealing in DP steel involves phase transformation at the microscale and the finite element simulation of this heat treatment could be greatly improved by such an ICME approach. In the present work, phase field modeling implemented in the software package Micress is used to simulate the microstructure evolution during inter-critical annealing. Asymptotic Homogenization is used to predict the effective macroscale thermoelastic properties from the simulated microstructure. The macroscale effective flow curves are obtained by performing Virtual Testing on the phase field simulated microstructure using Finite Element Method. All the predicted effective properties are then passed on to the macro scale FE simulation software Simufact Forming, where the heat treatment cycle for the

inter-critical annealing is simulated. The thermal profiles from this simulation are extracted and passed on to microscale to repeat the process chain. All the simulation softwares are integrated together to implement a multi-scale simulation, aiming towards ICME approach.

11:30 AM

Integrated Computational Materials Engineering Approach to Development of Lightweight Third Generation Advanced High-Strength Steel (3GAHSS) Vehicle Assembly: *Harjinder Singh*[1]; Mahendran Paramasuwom[1]; Vesna Savic[2]; Louis G. Hector, Jr.[2]; Ushnish Basu[3]; Anirban Basudhar[3]; Nielen Stander[3]; [1]EDAG, Inc.; [2]General Motors; [3]Livermore Software Technology Corp.

This presentation will cover an application of integrated computational materials engineering (ICME) for third generation advanced high-strength steels (3GAHSS) to vehicle lightweighting. Following a brief overview of the ICME project, design optimization of a vehicle structure using a multi-scale ICME material model will be presented. Preliminary results show 35% mass reduction potential of a mid-size sedan body side structure with the use of 3GAHSS. Design optimization steps, as well as the challenges in application of ICME models in vehicle design integration and optimization will be addressed. The presentation will conclude with integration steps that are needed to enable vehicle performance metrics driven material development in terms of chemical composition and phase characteristics.

11:50 AM

Integrated Microstructure based Modelling of Process-Chain for Cold Rolled Dual Phase Steels: *Danish Khan*[1]; Ayush Suhane[1]; Srimannarayana P[1]; Akash Bhattacharjee[1]; Gerald Tennyson[1]; Pramod Zagade[1]; B.P Gautham[1]; [1]TRDDC, TCS Research, Tata Consultancy Services

The properties of dual phase (DP) steels are governed by the underlying microstructure, the evolution of which is determined by the processing route. In order to design a dual phase steel with tailored properties, it is therefore important to model and design each of the process involved at the microstructure level in an integrated fashion. In this work, an integrated approach is used to predict the final microstructure and mechanical properties of dual phase steels through microstructure based modelling of cold rolling, intercritical annealing and quenching processes. Starting with a representative volume element (RVE) of initial ferrite-pearlite microstructure, cold-reduction during rolling is simulated in a FEM based micromechanics approach under appropriate boundary conditions. The deformed microstructure with plastic strain energy distribution after cold-reduction serves as input for modelling recrystallization and ferrite to austenite transformation during intercritical annealing using a phase-field approach. A micromechanics based quenching simulation is then used to model austenite to martensite transformation, related volume expansion and evolution of transformational stress/strain fields. The resultant microstructure with its complete state is used to evaluate the flow behavior under uniaxial loading conditions in a FEM based micromechanics approach under periodic boundary conditions. Property variation for different initial microstructure, composition and processing conditions are studied and discussed.

12:10 PM Lunch on Your Own

Additive Manufacturing - I

Monday AM
May 22, 2017

Room: Salon II, III
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

10:30 AM

Prediction of Microstructure, Residual Stress, and Deformation in Laser Powder Bed Fusion Process: *Yu-Ping Yang*[1]; Mahdi Jamshidinia[1]; Paul Boulware[1]; [1]EWI

A transient thermal-metallurgical-mechanical analysis method has been developed to predict temperature, microstructure, hardness, stress, strain, and deformation for Laser powder bed fusion (L-PBF). The analysis method includes a pre-processing module, a powder deposition module, a thermal module, a metallurgical module, and a mechanical module. The pre-processing module is used to slice a solid geometry into layers and create laser heat lines for each layer based on a designed scan pattern. The power deposition module is used to model powder-to-solid transition by changing material properties based on the laser's locations. The thermal module includes two heat-source models, a Goldak double-ellipsoidal model and a moving line heating model, which work with ABAQUS software to predict temperature by inputting laser power, travel speed, and a heat-line sequence. The metallurgical module is used to predict microstructure and hardness by inputting the predicted temperature history with the Goldak heat-source model. The mechanical module is used to predict stress and deformation by inputting the predicting temperature history with the line heat source model and modeling the melting effects. Microstructure and hardness of AISI 4140 steel built with L-PBF were predicted using the developed numerical modeling tool. Experimental measured hardness was used to validate the model prediction. It was found that tempering effect has to be modeled in order to predict the hardness correctly. Residual stress and deformation of Inconel 718 were predicted in a block sample built by L-PBF.

10:50 AM

Enabling Component-scale Prediction in Additive Manufacturing by Integration of Physics-based and Data-driven Modeling: Jingran Li[1]; Ran Jin[1]; *Hang Yu*[1]; [1]Virginia Tech

Additive manufacturing of materials often involves complex physical processes, such as light absorption and powder melting, dynamic melt flow, and rapid solidification, resulting in complex co-evolution of the thermal field, microstructure, and residual stresses. Owing to the multi-scale, multi-physics, and non-equilibrium nature of additive manufacturing, property prediction across the component has been challenging. For example, strategies remain elusive for identifying model discrepancies and unknown physical parameters, for reducing computation cost, and for quantifying modeling uncertainties. Here, we present a theoretical and experimental framework for component-scale prediction and uncertainty quantification, in which physics-based and data-driven models are integrated, and are validated by in situ thermal imaging and ex situ dimension measurement. 3D finite element modeling of the thermo-mechanical process captures the underlying physics; supervised machine learning-based surrogate models accelerate the computation speed; Bayesian calibration quantifies model discrepancies and parameter uncertainties. This framework enables property prediction on the component scale with different geometric designs, under different processing conditions, and at a low computation cost. These will be demonstrated in processes such as fused deposition modeling and directed energy deposition.

11:10 AM

Transforming Additive Manufacturing through Exascale Simulation: *James Belak*[1]; Wayne King[1]; John Turner[2]; Lyle Levine[3]; Neil Henson[4]; Neil Carlson[4]; [1]Lawrence Livermore National Laboratory; [2]Oak Ridge National Laboratory; [3]National Institute of Standards and Technology; [4]Los Alamos National Laboratory

Additive manufacturing (AM) offers the prospect of revolutionizing the fabrication of components and parts with unique properties. Despite this enormous potential, the insertion of AM parts has been limited due to the difficulty in qualifying parts. Starting from a top-down systems engineering approach, an integrated computational materials engineering (ICME) approach can be used to accelerate the qualification and adoption of newly additively manufactured parts by enabling up-front assessment of manufacturability and performance. Recently, we were awarded one of the USDOE Exascale Computing Project's Application Development Centers to create a new modeling framework for additive manufacturing amenable to exascale computing. The project includes an integration of all the computational components of the AM process into a coupled-exascale modeling framework, where each simulation component itself is an exascale calculation. In order to expose the physics fidelity needed to enable part qualification, the project is driven by a series of demonstration problems that are amenable to experimental observation and validation. In particular, in situ experiments on instrumented AM machines will be used to measure local material properties during build that give rise to macroscopic properties such as residual stress. Here, we present our coupled-exascale simulation framework for additive manufacturing and its initial application to AM builds.Work was performed under the auspices of the U.S. Department of Energy by LLNL, ORNL and LANL under contract DEAC5207NA27344.

11:30 AM

ICME Modules to Account for and Exploit Additive Manufacturing Process-Structure-Property Relationships in Component Design: *Michael Groeber*[1]; Edwin Schwalbach[2]; Michael Uchic[2]; Paul Shade[2]; Bill Musinski[2]; Sean Donegan[2]; Daniel Sparkman[2]; Jonathan Miller[2]; [1]AFRL; [2]Air Force Research Laboratory

Additive manufacturing presents both extreme potential and concern for component design. The ability to locally tailor processing path opens the door to sophisticated new designs with heterogeneous properties. However, accounting for this heterogeneity, before exploiting it, requires the ability to link local processing state to properties/performance of local material. A concern with current geometry-based design approaches, such as topology optimization, is not directly accounting for material property changes as geometry updates are made. Given current closed and fixed scanning strategies of most commercial systems, local processing paths are potentially altered significantly with seemingly minor macroscopic geometry changes and are unable to be avoided. This work intends to build ICME modules that predict microstructure (grain size, texture, void Vf, etc.) from processing history and predict performance (E, sys, hardening rate, ef, etc.) from microstructure. These modules will be designed to interface with topology optimization codes to dynamically account for material properties as geometry updates are made. The work is being demonstrated using a laser-based powder-bed fusion process on nickel superalloy IN625 for thin-walled structures. Highly-pedigreed data sets of in-situ monitoring data (beam path, thermal measurements), post-build characterization (CT, RUS, 3D Optical and SEM) and mechanical testing (milli-tensile, HEDM, notch and torsion testing) will be collected and provided to the open community. Challenges problems will be commissioned to benchmark the current modeling capabilities in process-structure and structure-properties. Finally, challenge results will be used in novel forecasting techniques akin to weather forecasting strategies of model aggregation.

11:50 AM

Influence of Computational Grid and Deposit Volume on Residual Stress and Distortion Prediction Accuracy for Additive Manufacturing Modeling: Mustafa Megahed[1]; Joerg Willems[1]; Pierre-Adrien Pires[1]; *Olivier Desmaison*[1]; [1]ESI Group

Powder Bed Additive Manufacturing offers unique advantages in terms of cost, lot size and complexity. The energy used however leads to distortions during the process. The distortion of single layers can be comparable with the powder layer thickness. The contact between the coater blade and the deposited material could terminate the build process. Furthermore, accumulated residual stresses can lead to deviations of the final shape from the design. Several residual stresses and distortion prediction models have been introduced and they have demonstrated qualitative agreement with expectations and experiments. All methods are based on assumptions and process simplifications – most of which were developed and confirmed for welding technology. The use of large deposits is justified by the acceleration of the computational procedure. This work focusses on the accuracy of quick residual stress and distortion models that will both provide layer by layer distortion data as well as the final work piece residual stress and shape. Different methods are utilized and compared in terms of accuracy and computation cost. The most promising model (instantaneous shrinkage approach) is further analyzed to determine conditions for accurate predictions. The residual stress and distortion models are implemented in an ICME platform that takes powder size distribution into account as well as the heat source powder interaction into account. Lower scale models are briefly introduced and data required for the residual stress analysis are documented prior to the analysis of some large components assessing manufacturability and final work piece shape.

12:10 PM Lunch on Your Own

Microstructure Evolution - I

Monday AM
May 22, 2017

Room: Salon IV
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

10:30 AM

SPPARKS - A Platform for Simulation of Material Microstructures: *Jonathan Madison*[1]; Theron Rodgers[1]; Veena Tikare[1]; [1]Sandia National Laboratories

Integrated Computational Materials Engineering (ICME) hinges upon the enabling interactions of simulation with experiments to hasten, improve and bolster the design cycle for materials. This requires simulation tools which are properly scoped, reliable and sometimes flexible to the need at hand. With regard to meso-scale microstructural predictions, few simulation codes currently exist which are readily extensible, maintain low computational overhead, are applicable to a variety of material phenomena and are also free of cost. However, Sandia's SPPARKS platform, which is an acronym for Stochastic Parallel PARticle Kinetic Simulator, is. This talk will present an overview as well as a few select user routines from within SPPARKS which provide first order approximations of microstructure undergoing coarsening, static or dynamic recrystallization, laser-welding and even additive manufacturing. Sandia National Laboratories is a multi-mission 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

10:50 AM

Extending CALPHAD Based Tools with Process-Structure-Property Models to Develop a Computational Materials Design Platform: *Johan Jeppsson*[1]; Adam Hope[1]; Kevin Wu[1]; Qing Chen[1]; Johan Bratberg[1]; Anders Engström[1]; Ralf Rettig[1]; [1]Thermo-Calc Software

CALPHAD is a phase based approach to describe the underlying thermodynamics and diffusion in complex, multicomponent systems taking into consideration composition and temperature variations. In the early days of CALPHAD, predictions were limited to thermodynamic equilibrium. The approach was then extended to consider diffusion controlled kinetics. More recently, development has focused on precipitation kinetics and also the modelling of microstructure evolution through phase field. This enables the predictive modelling of process-structure with variations in chemistries essential for materials design. The ultimate interest in materials design or Integrated Computational Materials Engineering (ICME) is understanding material properties or possibly performance, and to reach there we need process-structure-property relationships. 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 of property models and how Thermo-Calc users can implement own property models using the script language Jython(Python for Java VM). In addition, new functionality and infrastructure supporting computer aided materials design will be discussed and It will be shown how to visualize and export the results from property models.

11:10 AM

Microstructural Design of Thermal Sprayed Chromium Oxide Coatings: *Tatu Pinomaa*[1]; Tom Andersson[1]; Anssi Laukkanen[1]; Tomi Suhonen[1]; Jarkko Metsäjoki[1]; Nikolas Provatas[2]; [1]VTT Technical Research Centre of Finland; [2]McGill University

We present an approach to virtually design thermal spray coatings. Thermal spray coatings are deposited by melting and propelling micron-sized particles to a surface, resulting in a submillimeter-thick lamellar film. The coating microstructure forms via accumulation of rapidly solidified splats, which are modeled with a multi-order parameter phase-field model. A mesoscale finite-element model is then used to to relate microstructure properties–such as texture and interlamellar adhesion–to mechanical response of the coating. A set of simulated rapidly solidified chromium oxide microstructures are sampled to produce a complete synthetic coating. In addition, a set of scanning electron microscope (SEM) images are segmented and sampled to represent a coating volume. The simulation-based and SEM-based representations are compared: first their microstructural features, and second their mechanical properties. Finally, the simulation and SEM-based methods are combined to produce a richer representation of the coating. The lamellar and coating-substrate adhesion strengths tend to bottleneck the coating performance, and therefore these interface regions are treated with special care. The chromium oxide tends to reduce into metallic chromium, and the portion of chromium is varied to see its influence on the coating performance.

11:30 AM

Multi-Scale Modeling of Quasi-Directional Solidification of a Cast Si-rich Eutectic Alloy: Chang Kai Wu[1]; *Kwan Skinner*[1]; Andres Becerra[1]; Vasgen Shamamian[1]; Salem Mosbah[2]; [1]Dow Performance Silicones; [2]Think Solidification, LLC

Dow Corning Corporation recently examined the use of transition metal-silicon eutectics for producing melt-castable ceramic parts. These materials display good strength, wear and corrosion resistance. The near-eutectic solidification structure has significant impact on the final properties of a cast component. However, direct simulation of the cast structure at industrial scales remains a challenge. The objective of this work is to develop a multi-scale integrated solidification model that includes: density functional theory (DFT) calculations, which enable the computation of difficult-to-measure thermophysical properties; microstructural evolution simulation, which tackles nucleation eutectic growth and segregation during solidification; and casting modeling, which accounts for different boundary conditions including temperature-dependent heat transfer coefficients and geometry. The developed 3D coupled code can predict the correct morphology of the solidified composite and aid in the design and optimization of melt-cast parts based on composition and process parameters in a virtual environment. To verify the model, a mold was designed to achieve quasi-directional solidification within large regions of each casting; hypo- and hyper-eutectic Si-Cr alloys were cast into this custom mold using a vacuum tilt pour unit. Our experimental efforts focused on the quantification of the effects of process conditions on the resulting microstructure of the cast component. Local segregation was examined and compared with the model's predictions. Results are in agreement with the microstructure observed in our castings.

11:50 AM

A Model for Prismatic Grain Growth in Cemented Carbides: *Manon Bonvalet*[1]; Joakim Odqvist[1]; Annika Borgenstam[1]; John Ågren[1]; [1]KTH - Royal Institute of Technology

Cemented carbides, consisting of hard WC grains embedded in a ductile matrix (Co for instance), are used in the manufacturing industry, for e.g. cutting tools, thanks to an interesting combination of hardness and toughness. These mechanical properties are mainly due to the average grain size and the grain size distribution, and consequently the prediction of their evolution and the understanding of the physical phenomena driving it are of a great importance. Cemented carbides are made by liquid phase sintering and during this process abnormal grain growth may occur, i.e. few large grains of WC, consume the small neighbouring grains. This phenomenon cannot be explained in view of the classical LSW theory. The flat surface planes of the grains observed experimentally suggest that the grain coarsening is controlled by interface reaction. The 2D nucleation of new atomic layers on the different facets consumes a part of the driving force for coarsening. Our grain growth model deals with this 2D nucleation but also with the mass transfer across the interface and the long-range diffusion during growth. These phenomena are coupled in series. In addition, the prismatic grain shape and the anisotropic interfacial energy are taken into account. The driving force for coarsening, which is written for a non-spherical grain, is dissipated by different physical phenomena and the interfacial energy of different grain facets. A Kampmann-Wagner approach is used to describe the evolution of the grain size distribution within the system over time. Predictions are compared with experimental results for different multicomponent systems.

12:10 PM Lunch on Your Own

Integration Framework and Usage - IB

Monday PM
May 22, 2017

Room: Salon I
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

2:00 PM Invited

Center for Hierarchical Materials Design: Data and Databases for ICME: *Emine Gulsoy*[1]; Laura Bartolo[1]; Juan De Pablo[2]; Gregory Olson[1]; Peter Voorhees[1]; [1]Northwestern University; [2]University of Chicago

Center for Hierarchical Materials Design (CHiMaD) is a NIST-sponsored Center of Excellence for Advanced Materials Research, focusing on developing the next generation of computational tools, databases and experimental techniques in order to enable the accelerated design of novel materials and their integration to industry. Integrated computational materials engineering tools are vital for realization of the Materials Genome Initiative and CHiMaD is leading several fronts in data and proto-data development for both organic and inorganic materials. CHiMaD's prototype-data development will be discussed as well as its efforts in database development for organic and inorganic materials along with community initiatives including Data Workshops and Materials Data Facility which aims to serve as a community resource for sharing, storing and mining data.

2:30 PM

Integration of Experiments and Simulations to Build Material Big-Data: *Gunjin Yun*[1]; [1]Seoul National University

In this paper, a method for extracting stress-strain databases from material test measurements is introduced as one of the potential Integrated Computational Materials Engineering (ICME) tools. Measuring spatially heterogeneous stress and strain evolutionary data during material tests is a challenging and costly task. The proposed method can extract a large volume of spatially heterogeneous stress and strain evolutionary data from experimental boundary measurements such as tractions and displacements. For the purpose, nonlinear finite element models are intrusively implemented with artificial neural network (ANN)-based material constitutive models. Then a specialized algorithm that can auto-progressively train ANN material models guided by experimental measurements is executed. Any complex constitutive law is not presumed. From the algorithm, ANN gradually learns complex material constitutive behavior. The training databases are gradually accumulated with self-corrected stress and strain data predicted by the ANN. Finally, material databases are obtained. For an example, visco-elastoplastic material databases are obtained by the proposed method.

2:50 PM
ICME Based Hierarchical Design Using Composite Materials for Automotive Structures: Azeez Shaik[1]; Yagnik Kalariya[1]; Rizwan Pathan[1]; *Amit Salvi*[1]; [1]TCS Research, Tata Consultancy Services

Composite materials are increasingly being used in automotive structures due to their higher specific stiffness and specific strength. Composite material characterization is a complicated task due to micro-scale non-homogeneity and its resulting anisotropy and is generally accomplished with expensive physical tests at coupon level. High fidelity computational models are increasingly being used to accurately establish the elastic material behaviour that also provides detailed information about nonlinear behaviour due damage and fracture. The fiber architecture or composite microstructure can be altered to provide a maximum performance for a given application under certain loads. Thus, material selection from existing materials, and material design for a given component needs to be integrated in the existing design cycle.In this paper, ICME based hierarchical design process integrated with composite material selection and microstructure based material design will be presented. An automotive car door assembly will be designed using this approach. Material selection from given list of composite materials will be carried out using stiffness based approach. Individual components will be checked for damage and failure and a fiber reinforced composite material is designed specifically to suit the requirement keeping the overall stiffness very close to the global requirement. This framework for design decisions is integrated using a TCS PREMAP framework developed in house.

3:10 PM
Hot-tearing Modeling of Multicomponent Al-Cu Alloys in an Integrated Computational Materials Engineering Approach: *Adrian Sabau*[1]; Seyed Mirmiran[2]; Christopher Glaspie[2]; Shimin Li[3]; Diran Apelian[3]; Amit Shyam[1]; J. Haynes[1]; Andres Rodriguez[4]; [1]Oak Ridge National Laboratory; [2]Fiat Chrysler Automobiles North America; [3]Worcester Polytechnic Institute; [4]Nemak Monterrey

Hot-tearing is a major casting defect that is not a material property but rather a result of the combined effects of thermodynamic phenomena leading to phase precipitation at grain boundaries, solidification microstructure, inter-dendritic feeding, and stress evolution during solidification. The availability of constitutive models for the simulation of hot-tearing and the much longer computational times required for process simulations poses a challenge to the ICME models. The susceptibility of Al-Cu multicomponent alloys to hot-tearing during permanent mold casting was investigated using a constrained permanent mold in which the load and displacement was measured. The experimental results for hot tearing susceptibility are compared with those obtained from numerical simulations. The Cu composition was varied from approximately 5 to 8 pct. (weight). The data for the measured load and displacement during casting were compared with those obtained from numerical simulations to assess the current-state-of-the-art for hot-tearing modeling.

3:30 PM Break

3:50 PM
An Integrated Computational Model for Keyhole Laser Welding Process and Residual Stress Prediction: *Lili Zheng*[1]; Jiye Wang[1]; Wei Yuan[1]; [1]Hitachi America Ltd

An integrated computational modeling framework is being developed to simulate keyhole laser welding process and residual stress distribution in welded stainless steels. A conical Gaussian type heat source model is established to predict the temperature profile. As a prerequisite, extensive laser welding experiments are carried out to determine the heat input parameters in the model. For evaluation, the weld bead profile predicted from the heat source model is compared with that from experimental observation. The temperature profile from the heat source model is then passed onto the thermal-mechanical sub-model as thermal load in order to analyze the residual stress distribution in the welds. X-ray diffraction method is adopted to measure the residual stress and verify the model accuracy.

4:10 PM
Reduced-order Models for Microscale Plastic Strain Rate Fields in Two-phase Composites Subjected to an Arbitrary Macroscale Plastic Strain Rate using Data Science Approaches: *David Montes de Oca Zapiain*[1]; Evdokia Popova[1]; Surya R. Kalidindi[1]; [1]Georgia Institute of Technology

We will present a reduced-order (computationally fast) model that predicts the microscale spatial distribution of plastic strain rate in a two-phase composite subjected to an arbitrary macroscopically imposed strain rate tensor (using periodic boundary conditions). This model was developed using a recently developed framework of localization linkages called the Material Knowledge Systems (MKS). In prior work, the framework was successfully used to predict local strain rate fields in multiphase composites subjected to a given macroscale plastic strain rate. In the present work, the framework was extended to allow building these reduced-order models for the complete set of all macroscale plastic strain rates that could be applied at the macroscale. These reduced-order models (also called localization linkages) were calibrated and validated to results from microscale finite element models.

4:30 PM
Continuum Dislocation Dynamics Model of Heterogeneous Deformation in a Multimodal Particle Nickel Based Superalloy: *Joseph Rangel*[1]; Gavin Yearwood[1]; James Little[1]; Jonathan Benson[1]; Hector Basoalto[1]; [1]University of Birmingham

A continuum dislocation field plasticity framework has been developed to study heterogeneous slip development under cyclic loading conditions, accounting for multimodal particle distribution. The model simulates a continuum dislocation density (CDD) evolution through a gamma prime (γ') type dispersion on a 2D cross section of a single grain, and takes into account dislocation mobility and interaction. A non-local theory is used to represent the influence of long-range combined dislocation stress fields which influence the dislocation motion and behaviour at obstacles, observed through events such as climb and pile-up. The model strives to replicate the heterogeneous nature of plastic deformation. Simulations are carried out on a representative microstructure of high volume fraction disc Superalloy, which includes grain boundaries and multi modal distribution of gamma prime precipitate particles (γ'). The strain maps generated by the model are compared with experimental in-situ results.It is shown that large concentrations of localised deformation are identified as potential sites for fatigue crack initiation, once surpassing a critical value. This critical value is determined by the amount of shear that would indicate the opening of a micro-crack. The volume fraction particle size distribution of the gamma prime the microstructure is varied to see the influence on stress distribution and cyclic loading response. These results are analysed to see which precipitate particle distributions promote resistance to fatigue crack initiation.

Additive Manufacturing - II

Monday PM
May 22, 2017

Room: Salon II, III
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

2:00 PM Invited
Validation of Integrated Computational Materials Engineering Principles for Optimization of Fatigue Properties of Ti-6Al-4V Alloys Made by Laser Direct Energy Deposition: *Sudarsanam Babu*[1]; A. Prabhu[1]; N. Sridharan[2]; K. Makiewicz[3]; W. Zhang[4]; A. Chaudhary[5]; [1]The University of Tennessee, Knoxville; [2]Oak Ridge National Laboratory; [3]Formerly from The Ohio State University; [4]The Ohio State University; [5]Applied Optimization Inc.

In early 2000, Kobryn and Semiatin published a classic paper that showed the challenges associated with laser additive manufacturing of Ti6Al4V alloys in terms of anisotropic fatigue properties. The above deficiencies were attributed to tendency for the formation of physical defects that include porosity and lack of fusion, as well as, microstructural heterogeneity. In 2005, Kelly et al attributed the microstructural heterogeneities such as "white band" formation to cyclic phase transformations within the □+□ phase field. Although, these challenges were addressed through post-process hot isostatic pressing, the need for in-process control of microstructure was realized for complex geometries. In this talk, the step-by-step approach for developing computational tools for describing thermal gyrations and concurrent microstructure (solidification and solid-state transformation) evolution during laser additive manufacturing

will be discussed. This integrated model was used in a "numerical trial-and-error experimentation" and optimum conditions that led to homogeneous microstructure was selected. The processing conditions, which involved processing above transus, showed that it is indeed possible to arrive at homogeneous basketweave microstructure. Further process optimizations lead to improved fatigue properties without any post process heat treatments. In addition, the experimental data also showed uncertainties in ensuring fatigue properties with this ideal process parameter set. Such uncertainties were attributed to spatial location of defects and variability in performance of auxiliary equipments, such as powder flow. The feasibility of extending these tools for nickel base alloys was also explored. These results demonstrate that the ICME tools provide a viable pathway for rapid qualification of AM components.

2:30 PM

Mesoscale Multi-Physics Simulation of Solidification in Selective Laser Melting Process: *Dehao Liu*[1]; Yan Wang[1]; [1]Georgia Institute of Technology

Selective laser melting (SLM) is a powder bed based additive manufacturing process by melting fine-grained metallic powders with a laser heating source. Understanding the solidification of alloys during SLM process is of importance for accurate prediction of microstructures and properties for process optimization. In this study, a multi-physics based phase field model is developed to simulate evolution of alloy microstructure during solidification, which incorporates heat transfer, fluid dynamics, and kinetics of phase transformations and grain growth. The effect of cooling rate is investigated through simulation. The simulation results are compared with the morphology of dendrite from experimental measurement.

2:50 PM

Investigating the Role of Porosity in Additively Manufactured IN718 by Crystal Plasticity Modeling and Tomography Characterization: *Veerappan Prithivirajan*[1]; Todd Book[2]; Alexander Finch[1]; Michael Sangid[1]; [1]Purdue University; [2]US Military Academy

Direct metal laser sintering (DMLS) can be used for aerospace applications to realize numerous advantages, which have been well documented. However, prior to their use in safety critical components, the failure mechanisms have to be well understood, especially for the unique defects in DMLS materials, especially porosity. In our work, we study the critical pore size and volume fraction relative to the microstructure of a Ni-based superalloy, IN718, produced by DMLS via crystal plasticity finite element (CPFE) simulations and compare with synchrotron micro-tomography characterization results. 3D virtual microstructures with varying pore sizes and volume fractions are developed and subsequent cyclic simulations are carried out using a CP-FE framework. The critical size of the pore is defined as the size beyond which the crack nucleation transitions from crystallographic planes/GBs to the vicinity of the void. The crack nucleation site is influenced by many factors such as large grains, orientation distribution, grain neighbor interactions, twin boundaries, void size, and void interactions. Finally, the CPFE simulation results are compared with the porosity observed in DMLS IN718 via synchrotron micro-tomography characterization results.

3:10 PM

Precipitate Kinetics in Inconel 718 Additive Manufactured Components: *Magnus Anderson*[1]; Chinnapat Paniwisawas[1]; Yogesh Solvani[1]; Richard Turner[1]; Jeffery Brooks[1]; Hector Basoalto[1]; [1]University of Birmingham

A mean field model of the precipitation kinetics of the intermetallic particle phases in IN718 has been developed and applied to predict nucleation, growth, coarsening and dissolution behaviour during additive manufacture. The engineering properties of this alloy depend on the formation of a complex distribution of both metastable and equilibrium phases. Consequently, a simulation tool is needed to assist in the design of heat treatments to avoid excessive precipitation of the d phase and understand how the heat affected zone develops during additive manufacture. Svoboda et al's (2004) multi-component mean field particle coarsening model has been implemented. The approach is similar to that described by Zickler et al, 2010. The γ' particles are approximated to be spherical, whilst Kozeschnik et al's shape factors are used to describe the γ" and d phases by cylindrical discs. The interfacial energy and nucleation site density were calibrated to predict the precipitation kinetics of the γ" and d presented by Fisk et al (2014), Azadian et al (2004) and Beaubois et al (2004). The thermal history occurring within an ALM component during manufacture has been simulated using a Finite element model. The kinetics of precipitation resulting from the thermal loading have been simulated at a cross section of the component. The model predicts changes in particle dispersion across the heat affected zone, and also the repeated nucleation and dissolution of precipitates due to the repetitive passing of the heat source over the deposited material.

3:30 PM Break

3:50 PM

Large Scale Phase Field Simulations of Microstructure Evolution in POlycrystalline Ti-6Al-4V during Multiple Thermal Cycling: *Bala Radhakrishnan*[1]; Sarma Gorti[1]; Suresh Babu[1]; [1]Oak Ridge National Laboratory

The phase field method has been established as a standard ICME tool for simulating microstructural evolution during thermo-mechanical processing of structural alloys. The objective of this study is to perform large scale, high spatial resolution phase field simulations of the beta to alpha transformation in polycrystalline Ti-6Al-4V alloy during multiple thermal cycling, and to validate the simulation results using experimental microstructures generated during additive manufacturing of the alloy. The proposed simulations will be based on an extension of our recent work on isothermal simulations in single crystals using a novel composite nucleation model that demonstrated an intragranular mechanism for the formation of lamellar alpha in Ti-6Al-4V based on the interaction between the nucleation rate and the accommodation of strain energy associated with the beta to alpha transformation. The proposed simulations will address the combined effects of grain boundary nucleation and variant selection of alpha and intragranular nucleation of alpha on the morphology transition from basket-weave to lamellar alpha within the layer bands formed during additive manufacturing. Research at Oak Ridge National Laboratory is managed by UT-Battelle, LLC, under contract DE-AC05- 00OR22725 for the U.S. Department of Energy.

4:10 PM

A Phase Field-based Microstructure Evolution Model for Selective Laser Melting of Ti-6Al-4V: *Mehdi Amiri*[1]; Kai Wing Kelvin Leung[1]; Nagaraja Iyyer[1]; [1]Technical Data Analysis Inc.

Selective laser melting (SLM) is an innovative additive manufacturing (AM) technique which offers an opportunity to control local microstructure and mechanical properties of a part, by adjusting process parameters such as scan speed and power of laser. Optimization of such process parameters is important in order to ensure the mechanical properties of parts fabricated by SLM process meet design requirements. In this work, we present an integrated multi-scale computational framework for predicting thermal history and evolution of microstructure of Ti-6Al-4V using a phase field modeling approach. Thermal model includes transient heat transfer analysis of a single layer multi-track SLM process using finite element techniques while microstructure model utilizes thermal history as an input to simulate alpha phase formation and its dissolution for the given thermal history. Phase field equations are implemented to account for alpha phase dissolution with diffusion equations and alpha phase formation by a Johnson-Mehl-Avrami-Kolmorgorov nucleation and growth model. This combined approach is able to quantify the effect of thermal cycling on the as-deposited microstructure and predict the evolution of alpha phase fraction, which ultimately controls mechanical performances. Results for different laser scan speed and laser power are presented and discussed.

4:30 PM

A Coupled Framework for the Spatial Design of Shape Memory Functionality in NiTi Based Additive Manufacturing: *Luke Johnson*[1]; Kubra Karayagiz[1]; Ji Ma[1]; Brian Franco[1]; Gustavo Tapia[1]; Alaa Elwany[1]; Ibrahim Karaman[1]; Raymundo Arroyave[1]; [1]Texas A&M University

The ability to precisely control part geometry and functional grading are the two most common examples of fabrication freedom granted by additive manufacturing that are not commonly attained through other more conventional manufacturing approaches. However, there are more dimensions in the design space that remain to be explored. This talk will describe a framework for precipitation design in NiTi shape-memory alloy systems fabricated via SLM. The framework couples finite-element thermal modeling simulations with a thermodynamic and kinetic based precipitate evolution model to predict precipitate volume fraction in a fabricated part. The thermal model was calibrated against experimental pyrometer data and the precipitation model was calibrated against experimental data from the literature using Bayesian calibration techniques. While originally developed to help explain within-part spatial variations in shape-memory behavior, this model can be inverted to provide top-down spatial design of shape-memory functionality.

4:50 PM

Measurement and Calculation of Liquid Ti Alloy Properties with Application to 3D Printing: *Jonathan Raush*[1]; Brian Novak[2]; Xiaoman Zhang[2]; Dorel Moldovan[2]; Wenjin Meng[2]; Shengmin Guo[2]; [1]University of Louisiana at Lafayette; [2]Louisiana State University

Accurate high-temperature thermophysical property data for liquid metals and alloys are important for the development of realistic simulations of laser-based 3D printing processes. We are using an approach combining electrostatic levitation (ESL), molecular simulation, and CALPHAD calculations to obtain such data for Ti alloys. We performed vacuum ESL measurements with a container-less oscillating drop technique at NASA MSFC on molten elemental Ti, Ti-xAl binaries (x = 0-10% wt.), Ti-6Al-4V, and Ti-6Al-4V-10Mo which showed improved mechanical properties compared with traditional ß Ti alloys. We used classical molecular simulations to obtain densities, pair distribution functions, diffusivities, viscosities, surface tensions, and vapor pressures for Ti-xAl. The viscosity and surface tension results for pure Ti agree well with the ESL data while the Ti-xAl results show the same trends as the ESL data, but not always quantitative agreement. Chemical activity and Gibbs free energy of Ti-10Al were generated through the CALPHAD technique and compared to experimental values.

Microstructure Evolution - II

Monday PM
May 22, 2017

Room: Salon IV
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

2:00 PM Invited

Process Simulation and Experimental Investigation of Material Properties in Aluminum Resistance Spot Welds: Sainan Wu[1]; *Bita Ghaffari*[2]; Elizabeth Hetrick[2]; Mei Li[2]; Zhihong Jia[1]; Qing Liu[1]; [1]Chongqing University; [2]Ford Motor Company

Resistance spot welding (RSW) is a key joining technique in numerous industries. Though ubiquitous in the automotive industry, the vast majority of resistance spot welding production and research have been conducted on steel. The current emphasis on lightweighting has greatly increased the interest in fully understanding the influence of the process on RSW of aluminum alloys. In the present study, a variety of experiments and simulations have been conducted to characterize the microstructure and property evolution of AA6111 RSW. In addition to the traditionally-observed heat-affected zone, the presence of a few-millimeter wide thermo-mechanically affected zone (TMAZ), which lies between the weld nugget and base metal and is notably harder than both, is established and explored. The impact of two hardening mechanisms, strain hardening induced by the compressive force from the welding electrodes and precipitation hardening, are investigated. The evidence establishes that the formation of the TMAZ is dominated by strain hardening.

2:30 PM

Effect of Microsegregation on the Microstructural Banding in Manganese Steels - An Integrated Multiscale Approach: Himanshu Nirgudkar[1]; Saurabh Mangal[1]; Savya Sachi[1]; Surya Ardham[1]; Sagar Salunke[1]; Ayush Suhane[1]; Srimannarayana Pusuluri[1]; Rishabh Shukla[1]; Danish Khan[1]; Pramod Zagade[1]; Gautham BP[1]; *Gerald Tennyson Peter*[1]; [1]TCS Research, Tata Consultancy Services Limited

Microstructural banding is a major concern in wrought manganese steels, that occurs after hot rolling, in regions where austenite grain size is less than the wavelength of Mn microsegregation. The signature of microsegregation on banding and thereby on properties is a multiscale problem, which may be brought out significantly using an integrated multiscale modelling approach from casting to phase transformation at the run out table (ROT). In this study, a method is proposed to quantify microsegregation using a computational thermodynamics (CALPHAD) approach, with temperature and composition distribution as inputs from casting simulations. The microsegregation parameter along with grain size distribution from hot rolling are used as inputs for predicting phase transformation in ROT using a phase-field approach. Finite element based micromechanics approach is then used for predicting the mechanical properties of the microstructure. Structure-property relationships as a function of microsegregation and austenite grain size are obtained for an ensemble of microstructures. This established relationship of microsegregation - grain size - structure - properties will be used for predicting the locations of banding and variation of properties of a hot rolled strip through the microsegregation parameter.

2:50 PM

Numerical Simulation of Macrosegregation in a 535 Tons Steel Ingot with a Multicomponent-Multiphase Model: *Chen Kangxin*[1]; Tu Wutao[2]; Shen Houfa[1]; [1]Tsinghua University; [2]SMIC Advanced Technology Research & Development (Shanghai) Corporation

To accurately simulate the formation of macrosegregation, a major defect commonly encountered in large ingots, solidification researchers have developed various mathematical models and conducted corresponding steel ingot dissection experiments for validation. A multicomponent and multiphase solidification model was utilized to predict macrosegregation of steel ingots in this research. The model described the multi-phase flow phenomenon during solidification, with the feature of strong coupling among mass, momentum, energy, concentration conservation equations. Impact factors as thermo-solutal buoyancy flow, grains sedimentation, and shrinkage-induced flow on the macroscopic scale were taken into consideration. Besides, the interfacial solute constraint relations were derived to close the model by solving the solidification paths in the multicomponent alloy system. The phase diagrams of the multicomponent alloy system were determined by Thermal-Calc Software. Thus the impact of multicomponent on macrosegregation was considered. A finite-volume method was employed to solve the governing equations of the model. In particular, a multi-phase SIMPLEC (semi-implicit method for pressure-linked equations-consistent) algorithm was utilized to solve the velocity-pressure coupling for the specific multiphase flow system. Finally, the model was applied to simulate the macrosegregation in a 535 tons steel ingot with composition of Fe-0.24 wt.%C-1.65wt.%Cr-1.39wt.%Mo. The simulated results were compared with the experimental results. Predictions have reproduced the macrosegregation patterns in measurements. A good agreement is shown generally in quantitative comparisons between experimental results and numerical predictions of carbon, chromium and molybdenum. It is demonstrated that the multicomponent multiphase solidification model can well predict macrosegregation in steel ingots and help optimize the ingot production process.

3:10 PM

Validation of CAFE Model with Experimental Macroscopic Grain Structures in a 36-ton Steel Ingot: *Jing'an Yang*[1]; Zhenhu Duan[2]; Baicheng Liu[1]; Houfa Shen[1]; [1]Tsinghua University; [2]Lishui University

In order to recognize macroscopic grain structures evolution within large heavy casting, a 36-ton steel ingot has been experimentally investigated. Fourteen thermocouples have been used to record temperature variations during solidification of the ingot to ensure a reliable simulation of temperature field.

Half of the longitudinal section has been etched to obtain as-cast macrostructure. Fine equiaxed grains are found in the ingot periphery, then slender columnar grains next to them, finally widely spread coarse equiaxed grains in the ingot center. Besides, several etched bands are detected which may be A-segregation channels. Then, simulation of macroscopic grain structure is processed by a three dimensional Cellular Automaton Finite Element(CAFE) module of ProCAST software. The nucleation algorithm is based on an instantaneous nucleation model considering a Guassian distribution of nucleation sites proposed by Rappaz. Besides, the growth algorithm is based on the growth of an octahedron bounded by (111) faces and the growth kinetics law is given by the model of Kurz et al. The microscopic CA and macroscopic FE calculation is weak coupled where the temperature of each cell is simply interpolated from the temperature of the FE nodes using a unique solidification path at the macroscopic scale. Simulation parameters of CAFE about Guassian nucleation and growth kinetics have been adjusted so that the macroscopic grain structures correlate with the as-cast macrostructure experiment.

3:30 PM Break

3:50 PM

Integrated Approach for Modelling of Precipitate Evolution and Grain Growth in Steel Slabs: *Saurabh Mangal*[1]; Himanshu Nirgudkar[1]; Savya Sachi[1]; Gerald Tennyson[1]; [1]TRDDC, TCS Research, Tata Consultancy Services

Micro-alloying elements such as Nb, V and Ti are added in steels to pin grain boundaries through precipitation and solute drag effect. Formation and dissolution of precipitates in casting and reheating, significantly impact further downstream operations. In this study, an integrated multiscale approach to capture the precipitation kinetics of vanadium carbonitrides V(C,N) during casting and reheating is proposed. The formation of precipitates depend on localized variation in composition due to microsegregation and dendrite arm spacing. Evolution of V(C,N) is predicted using temperature and composition distribution as input from macroscale casting simulations. The subsequent dissolution during reheating is modelled based on temperature evolution in the reheating furnace and is coupled to a cellular automata (CA) model simultaneously which takes inputs from CALPHAD calculations and predicts grain size evolution taking into account the grain boundary pinning effect due the presence of V(C,N). Precipitate evolution and dissolution for various processing parameters such as casting speed, superheat, reheating temperature and time are studied.

4:10 PM

Analysis of Localized Plastic Strain in Heterogeneous Cast Iron Microstructures using 3D Finite Element Simulations: *Kent Salomonsson*[1]; Jakob Olofsson[1]; [1]Jonkoping University

The design and production of light structures in cast iron with high static and fatigue performance is of major interest in e.g. the automotive area. Since the casting process inevitably leads to heterogeneous solidification conditions and variations in microstructural features and material properties, the effects on multiple scale levels needs to be considered in the determination of the local fatigue performance. In the current work, microstructural features of different cast irons are captured by use of micro X-ray tomography, and 3D finite element models generated. The details of the 3D microstructure differ from the commonly used 2D representations in that the actual geometry is captured and that there is not a need to compensate for 3D-effects. The first objective with the present study is to try and highlight certain aspects at the micro scale that might be the underlying cause of fatigue crack initiation, and ultimately crack propagation, under fatigue loading for cast iron alloys. An approach is implemented using cohesive elements to enable crack propagation in the microstructure simulations, and the simulation results are compared to 2D observations using Digital Image Correlation (DIC). The second objective is to incorporate the gained knowledge about the microstructural behaviour into multi-scale simulations at a structural length scale, including the local damage level obtained in the heterogeneous structure subjected to fatigue load.

4:30 PM

Crystal Plasticity Modelling of Martensitic Microstructures: Matti Lindroos[1]; Tom Andersson[1]; *Anssi Laukkanen*[1]; [1]VTT Research Center of Finland

Martensitic steels are widely used in many applications due to their high strength and reasonable ductility. The microstructural design of the martensitic steels plays an essential role in their suitability for different loading conditions varying from hostile wear environments in mining to fatigue engaging machine and transmission parts. The ICME approach on these microstructures requires the envisagement of the most important microstructural features as well as suitable numerical method to describe the deformation behaviour at the suitable length-scale. Lath martensite includes different identifiable length-characteristics such as prior austenite grains and its subfeatures packets, blocks and fine-sized laths, which all can contribute to material performance. However, in spite of the high engineering demand of martensitic steels, little attention has been placed in the modelling assisted development of the martensitic microstructures. One major reason for this is in the complexity in representing the morphologies and their dependencies, which easily leads to over-simplifications of the microstructures. We employ finite element crystal plasticity method on realistic martensite aggregates to investigate the performance of the martensitic microstructures under fatigue conditions. The results showed that the microstructure is length-scale sensitive originating from the fine martensite morphologies. The lifetime predictions of the material performance was also evaluated by interconnecting microscopic and macroscopic scales, while it was found that modifying the actual microstructure can improve material's performance. These results lay a foundation for the development of the design tools for martensitic microstructures.

Mechanical Performance Using Multi-Scale Modeling

Tuesday AM
May 23, 2017

Room: Salon I
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

8:00 AM

Scaling from Mesoscale to Macroscale in Viscoelastic Random Composites: Jun Zhang[1]; *Martin Ostoja-Starzewski*[1]; [1]University of Illinois

Microstructural randomness is one of basic characteristics of most solid materials. It affects their mechanical responses through properties of microconstituents, microstructural geometry, and scale of observation. While the macroscopic (homogeneous) continuum description of a material relies on the so-called Representative Volume Element (RVE i.e., macroscale level), the issue studied herein is the scale-dependent trend to it via a Statistical Volume Element (SVE, i.e. mesoscale level) in composites with linear viscoelastic, perfectly-bonded microconstituents, focusing on the quasi-static properties in the time as well as frequency domains. Requiring the material statistics to be spatially homogeneous and ergodic, the mesoscale bounds on RVE response are developed from the Hill-Mandel homogenization condition adapted to viscoelastic materials. The bounds are obtained from two stochastic initial-boundary value problems set up, respectively, under uniform kinematic and traction boundary conditions. The frequency and scale dependencies of mesoscale bounds are obtained through computational mechanics for composites with planar random checkerboard microstructures. In general, the frequency dependent scaling to RVE can be described through a complex-valued scaling function, which generalizes the concept originally developed for linear elastic random composites. This scaling function is shown to apply for all different phase combinations on random checkerboards and, essentially, is only a function of the microstructure and mesoscale.

8:20 AM

Strategy for Coupling Lengthscales for using Predictive Computation in Polymer Development for Mechanical Performance: *Steve Christensen*[1]; E Sharp[2]; [1]Schrodinger; [2]e-Xstream Engineering

Polymers for use as high performance engineering materials dates to the 1960's. Nearly all of the development of polymer composite materials has been empirical. Even with the recent emergence of molecular dynamics (MD) technology for simulation of polymer chemistry and advances in finite element analysis (FEA) simulation at the continuum level, development of new materials still largely depends on the traditional empirical approach. A key obstacle to materials development via simulation is the difficulty in linking simulation lengthscales from atomic (MD) through micromechanics to continuum. A physics based method utilizing the deformation modes of dilatation and/or distortion will be shown to provide new insight into polymer formulation. The method is a hierarchical multi-scale approach that relies on a new continuum analysis concept referred to as "Onset Theory" to provide the macroscopic guidance for polymer ultimate behavior leading to a new formulation. Condensed matter physics provides additional insight in how deformation is influenced by intra and intermolecular forces within covalently bonded polymeric materials. The method was first developed for use in describing behavior of composites. In addition, Molecular Dynamics can be of use to simulate the influence of small penetrant molecules and temperature on elastic properties leading to an inference on environmental resistance. We will show that a multiscale computational system using Molecular Dynamics, micromechanics modeling, and Onset Theory continuum modeling, with an appropriate protocol, can be used to perform virtual formulation and will yield results suitable for guiding materials development, leading to experiment and polymer evaluation demonstrating a performance improvement

8:40 AM

Hybrid Hierarchical Model for Damage and Fracture Analysis in Heterogeneous Material: *Alex Vasenkov*[1]; [1]Sunergolab Inc

Predictive damage and fracture analysis of heterogeneous material is grueling as such material consists of mesoscale components of different size and functionality. A logical approach taken by many researchers in tackling this challenge is to employ a framework that couples Molecular Dynamic (MD) and Finite Element (FE) modeling in some manner to capture damage processes occurring at different time and length scales. Unfortunately, such coupling typically suffers from lack of thermodynamic consistency between MD and FE models and the phenomena of pathological wave reflection, which occurs at the interface between MD and FE simulation regions. This works attempts to circumvent this problem with a Hybrid Hierarchical Model (HHM) involving an ab-initio based ReaxFF MD module and a peridynamic continuum module. The HHM framework was applied to perform damage and fracture analysis in a silicon carbide slab with pre-crack. The ReaxFF modeling was conducted around the crack region where the mechanical strains were the greatest and the most detailed resolution and the highest accuracy were required to predict the crack path. Peridynamic simulation was performed with increasing scale to provide more smeared and continuum-like solution for the crack path and capture correctly the waves caused by the crack propagation. The HHM was able to provide an atomistic-based description of damage and fracture mechanisms without contamination with pathological re□ections of waves from the MD boundaries, which are difficult to account in traditional MD simulation because of severe limitations on the size of simulation domain.

9:00 AM

Development of Integrated Computational Materials Engineering (ICME) Approach for Compression-Molded Chopped Carbon Fiber Sheet Molding Compounds (SMC) in Vehicle Light-weighting Applications: *Yang Li*[1]; Hongyi Xu[1]; Zhangxing Chen[2]; Danielle Zeng[1]; Jeffery Dahl[1]; Mansour Mirdamadi[3]; Xuming Su[1]; [1]Ford Motor Company; [2]Chongqing University; [3]The Dow Chemical Company

While the applications of continuous carbon fiber composites have been widely seen in many industries, chopped carbon fiber sheet molding compounds (SMC) made through compression molding process, featuring improved balance between weight reduction, mechanical properties and manufacturing cost, is regarded as an alternative promising material system for light-weighting products in automobile industry. However, the inhomogeneous and anisotropic mechanical behavior of the material hinders its deployment in vehicle part design. Furthermore the material properties are observed to be highly sensitive to the processing conditions, creating additional challenges for real-life applications. In the present study, an Integrated Computational Materials Engineering (ICME) approach is applied to develop a modeling framework which enables the computer-aided optimal design of the carbon fiber SMC parts without the necessity of performing a massive number of experiments in traditional trial-and-error procedures. The simulation of compression molding process realized in Autodesk Moldflow provides local microstructure information of the SMC material, which is then utilized in a multi-scale material modeling tool and generates homogenized material properties for macroscopic structural finite element analysis (FEA) to predict the part performance. Validations of the ICME models at different stages are provided through comparison between modeling prediction and experimental measurements. The workflow is automated with assistance from homemade MATLAB scripts and embedded into an optimization platform built in Esteco modeFrontier. An exemplar optimal design procedure on a vehicle subframe utilizing the developed ICME models is demonstrated.

9:20 AM

Automated Composite Material Model Development with Multiscale Designer: *Colin McAuliffe*[1]; Robert Crouch[1]; Jeff Wollschlager[1]; Jacob Fish[2]; Venkat Aitharaju[3]; Roger Ghanem[4]; [1]Altair Engineering Inc; [2]Columbia University; [3]General Motors Company; [4]University of Southern California

Development of accurate computational models for composite materials presents a challenge for industry practitioners. The input parameters to a multiscale model of a composite are the properties of the constituent materials, e.g. carbon fiber and epoxy. It is often not possible to fully characterize a complex constituent material like carbon fiber from performing experiments on them individually. Even if it were, manufacturing processes may result in different in situ properties. Model development therefore must be accomplished through inverse identification, where experimental observations on the composite are used with a model to infer the constituent properties. This presents its own set of challenges, since inverse problems are notoriously difficult to solve correctly. Additionally, the success of the inverse solution requires that each of the constitutive properties be constrained by at least one experimental observation. Due to the expense associated with testing of composites, there is strong motivation to minimize the number of tests.Multiscale Designer employs both deterministic and stochastic approaches to the model development problem for linear and nonlinear property identification. These approaches are automated and highly accessible to practicing engineers. The stochastic approaches provide crucial insight into the reliability of the inverse solution, and can inform the analyst when the lack of a particular experimental observation negatively impacts this solution. In this case, a purely deterministic approach may give the false impression of a good solution. In this presentation, the technical details of these approaches are presented, and their ability to successfully identify composite properties is demonstrated.

9:40 AM

Creep Damage Calculation of Weld Joint of 9Cr-1Mo-V-Nb Steel Tube for Creep Lifetime Prediction: *Kozo Koiwa*[1]; Masaaki Tabuchi[1]; Masahiko Demura[1]; Takaaki Matsuoka[2]; Keisuke Torigata[2]; Masayoshi Yamazaki[1]; Makoto Watanabe[1]; [1]National Institute for Materials Science; [2]IHI Corporation

Prediction of creep lifetime for weld joint of 9Cr-1Mo-V-Nb steel (ASME Gr. 91) tube was conducted by using computational simulation. The creep lifetime was predicted from the creep damage accumulation computed with the creep parameters obtained from the creep tests of base metal and heat-affected zone. Two type of creep damage mechanics analyses were applied, as follows: The Hayhurst-type analysis and the time exhaustion analysis assuming Norton creep law. The computed creep lifetime was compared with the experimental results to investigate the prediction accuracy of the computational creep simulation with the module can assess the creep lifetime of structural parts including varied materials.

10:00 AM Break

10:30 AM

Understanding the Role of Chemical Composition in the Formability and Mechanical Properties of Ni-base Superalloys: *Enrique Galindo-Nava*[1];

Catherine Rae[1]; [1]University of Cambridge

Nickel-base superalloys are widely employed in high-temperature structural components due to their excellent mechanical and environmental properties. These features can only be achieved by tailoring sophisticated microstructures through different thermomechanical routes, which are usually tailored for specific alloying contents. This work presents a systematic study on the role of chemical composition in the hot deformation and mechanical properties of Ni-base superalloys. A number of modelling strategies are integrated as a function of chemical composition to link microstructure evolution with tensile and creep strength. Evolution equations for dynamic recrystallization and grain growth including multicomponent solute drag and particle pinning are presented; it is explored how typical alloying elements present in superalloys affect the strain to reach complete recrystallization, altering the processing window of a component. An overview of compositional effects in precipitation evolution using existing simulation tools is presented. Microstructure-sensitive models for yield and creep strength developed recently are also introduced. The models are based on estimating the relative strengthening contributions of solid solution, grain boundary and multimodal particle shearing. The chemistry not only dictates the strength of each constituent but it also affects the values of interfacial energies; the latter alter the occurrence of different deformation mechanisms. The methodology is applied to identify optimal processing routes for improving mechanical properties in commercial Ni-base superalloys.

10:50 AM

A Strain Energy Based Damage Model for Fatigue Crack Initiation and Growth: *Peter Huffman*[1]; [1]John Deere

A strain energy based fatigue damage model is proposed which uses the strain energy from applied loads and the strain energy of dislocations to calculate stress-life, strain-life, and fatigue crack growth rates. Stress ratio effects intrinsic to the model are discussed, and parameterized in terms of the Walker equivalent stress and a fatigue crack growth driving force. The method is then validated using a variety of different metals with strain-life data and fatigue crack growth rate data available on the SAE Fatigue Design & Evaluation subcommittee database.

11:10 AM

Image-based Micromechanical Fatigue Simulation of Cast Aluminum Alloy by Parallel Finite Element Method: *Osamu Kuwazuru*[1]; Masaki Teranishi[1]; Shota Gennai[1]; Masataka Uchida[1]; Masakazu Kobayashi[2]; Hiroyuki Toda[3]; [1]University of Fukui; [2]Toyohashi University of Technology; [3]Kyushu University

Low-cycle fatigue test of cast aluminum alloy and its in-situ observation were performed in the synchrotron radiation facility SPring-8. The inclusions such as silicon and intermetallic particles were visualized by the X-ray CT. The crack initiation site and the particle of crack source were identified by the chronological CT observation. Then, the particle fracture life was also determined. A variety of the particle shapes and the particle fracture lives were selected, and the micromechanical finite element model of those particles was semi-automatically constructed with a lot of surrounding particles by the image-based modeling technique. The cyclic loading corresponding to the actual load in the experiment was applied to the finite element model. The material nonlinearity and the geometrical nonlinearity was considered, and the kinematic multi-linear hardening law was employed. Since the number of elements exceeded a ten million, we adopted a massively-parallel computing with a PC cluster system. Through these simulation results, the fatigue crack initiation mechanism and the effect of particle shape and distribution on the particle fracture life were discussed.

11:30 AM

Fatigue Performance Prediction of Structural Materials by Multi-Scale Modeling and Machine Learning: *Takayuki Shiraiwa*[1]; Fabien Briffod[1]; Yuto Miyazawa[1]; Manabu Enoki[1]; [1]The University of Tokyo

Structural materials having higher performance in strength, toughness, and fatigue resistance are strongly required. In the conventional materials development, many fatigue tests need to be conducted to validate statistical behavior of fatigue failure. Accordingly the evaluation of fatigue properties with shorter time becomes quite essential. Based on such background, we are developing fatigue prediction methods for wide range of structural materials by multi-scale finite element analysis (FEA) and machine learning. The multi-scale FEA consists of the following procedures: i) mechanical and thermal properties are estimated by using commercially available software and database; ii) temperature field, residual stress and distortion generated during a manufacturing process is calculated on the macroscopic model by thermo-mechanical FEA; iii) macroscopic stress field under cyclic loading condition is calculated with a hardening constitutive model; iv) the microscopic stress field is derived by finite element model with the polycrystalline structures and the cycles for a fatigue crack initiation is analyzed by Tanaka-Mura model; v) the cycles for fatigue crack propagation is analyzed by extended finite element method (X-FEM) and the total number of cycles to the failure is obtained. The second approach is to use empirical equation and fatigue database accumulated over the years. Materials and fatigue data have been aggregated from public databases, published papers and academic resources. Several empirical equations have been derived by applying machine learning techniques to the database. The accuracies and the features of our prediction methods will be discussed.

11:50 AM

Multiscale Modeling of Deformation Response of Polycrystalline Alloys using Orientation Distribution Functions: *Ali Ramazani*[1]; Veera Sundararaghavan[1]; [1]University of Michigan

An ICME approach to model texture evolution and mechanical behavior of polycrystalline alloys during deformation processing is presented. EBSD measurements were made in all surfaces (L-LT, L-ST and LT-ST) of samples in forged and compressed specimens. We have quantified the percentage of recrystallization in the forged specimens as well as the heat treated ones using grain orientation spread maps. Based on the experimental results, an orientation distribution function (ODF) model is developed to simulate the texture evolution at different intermediate strains in various loading conditions. Here, the polycrystalline microstructure is represented through a finite element discretized orientation distribution function and texture evolution is modeled using ODF conservation laws via Taylor assumption. Additionally, an elasto-visco plastic crystal plasticity framework is utilized to predict crystal reorientation. The ODF model is coupled to every integration point in a macro-micro Lagrangian finite element algorithm to predict the deformation response of the bulk material under compression. The approach results in a multiscale prediction where texture evolution is identified at every point in the macro-specimen. The ODF model is fully coupled to the macroscale mesh and can be used to predict spatial distribution of texture components. Numerical results show very good agreement with the experimental texture measurements.

12:10 PM Lunch on Your Own

Microstructure Evolution - III

Tuesday AM
May 23, 2017

Room: Salon II, III
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

8:00 AM

Microstructure Recognition and Analysis by Advanced Machine Learning: *Yoshitaka Adachi*[1]; [1]Kagoshima University

Human being can recognize a microstructure of metals and then extract its features manually based on standard metallography method. It is very important for metallurgists to understand correlation between a microstructure and a property. However it seems time-consuming to analyses microstructures by hand. The process how human being gets information from micrographs should be clarified to replace the role of human being with of computer on microstructure recognition. This study made an attempt to apply deep learning to quantify microstructures. An approach to microstructure quantification by convolutional neural network and advanced image processing will be demonstrated.

8:20 AM

The Microstructural Role: A Size Effect Approach: *Daniel Rodriguez Galan*[1]; Javier Segurado[1]; Ignacio Romero[1]; [1]IMDEA Materials

A vast and long-standing body of experimental evidence conclusively establishes the fact that the yield strength of crystals is size-dependent. This size dependence can be exploited to fabricate materials combining both high strength and ductility, e.g., by the equal channel angular pressing (ECAP) process (Rodríguez-Galán et al, 2015), and in other ways. In order to optimize the beneficial properties of grain refinement, it is necessary to understand the deformation micromechanisms governing the mechanical behaviour. These mechanisms depend on the refined grain size and also on other microstructural features, such as grain boundaries state, defect densities and crystallographic texture. However, the grain size plays a fundamental role. At this moment, non-local theories allow us to capture the size effect. However, these theories present a lot of challenges that are necessary to solve. We present an approach based on non-local theories with the objective to obtain the size effect in a natural way, to emphasize on numerical part of the problem.

8:40 AM

An Integrated Solidification and Heat Treatment Models for Predicting Mechanical Properties of Cast Aluminum Alloy Component: *Chang Kai Wu*[1]; Salem Mosbah[2]; [1]Dow Performance Silicones; [2]Think Solidification

In this work, a newly developed modeling tool is presented which computes the local mechanical properties of cast and precipitation hardening heat treated aluminum alloy component. The integrated model simulates both casting and heat treating processes, and it computes the local hardness, yield strength and ultimate tensile strength, that developed in the casting during each step. Both alloy solidification and precipitation hardening heat treatment steps are simulated. The solidification model takes into account grains nucleation and the mushy zone front undercooling to predict the growth of the dendritic and eutectic microstructures. The predicted secondary dendrite arm spacing (SDAS) map is used to calculate the local strengths in the subsequent heat treatment steps. The heat treating model takes into account quenching and aging steps. The integrated model uses an extensive database that was developed specifically for the A356 alloy under consideration. The database includes temperature dependent mechanical, physical, and thermal properties of the alloy.

9:00 AM

Modelling and Experimental Characterization of Microstructure Evolution during Cooling Stage of Homogenization Heat Treatment of Al-Mg-Si Alloys: *Qiang Du*[1]; [1]SINTEF

A CALPHAD-coupled multi-component multi-phase Kampmann-Wagner Numerical modelling framework, implemented in the software called PreciMS, has been employed to predict the precipitation of the stable and metastable phases, i.e., ß (Mg2Si) and ß' (Mg18Si10) during the cooling process within a homogenization heat treatment of AA6xxx alloys. The model is able to treat the concurrent nucleation and growth of the multiple phase particles during this non-isothermal process, and predict the evolutions of the precipitating particles' size distribution and fraction. The model predictions have been validated by the microstructure characterization carried out with Optical Microscopy, Scanning Electron Microscopy, Transmission Electron Microscopy and Electrical Resistivity Measurement on the samples from some dedicated homogenization heat treatment experiments of AA6xxx alloys. It is concluded that the proposed model is a valuable tool in optimizing and designing alloy chemistries and cooling process parameters.

9:20 AM

Precipitates Strengthening using Dislocation Dynamics: *Sylvie Aubry*[1]; Tom Arsenlis[1]; [1]LLNL

Predicting the influence of precipitate characteristics on the strength of selected aluminum-lithium alloys for a variety of heat treatment conditions has important applications for the aircraft industry. Currently, aircraft hybrid fan blades are made of titanium. Replacing these blades by aluminum-lithium alloys has been shown to lead to great savings in fuel consumption. The ability to model and predict the mechanical response of these alloys as a function of material processing parameters allows optimization of current forgings and future designs. As part of a multiscale approach the dislocation dynamics method has been used to predict the strength of materials. An extension of the dislocation dynamics method is presented. It takes precipitates into account. Interactions of dislocations defect with ellipsoidal precipitates is modelled. Large scale simulations of theta prime and T precipitates are presented. The stress/strain response as a function of precipitate characteristics are shown and explained. Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under ContractDE-AC52-07NA27344.

9:40 AM

Mutiscale Modelling of θ' Precipitation during Aging of Al-4wt.%Cu Alloys: Hong Liu[1]; Gustavo Esteban-Manzanares[1]; Bárbara Bellón[1]; Ilchat Sabirov[1]; *Javier LLorca*[2]; [1]IMDEA Materials Institute; [2]Polytechnic University of Madrid/IMDEA Materials Institute

The strength of Al-Cu alloys is controlled by the size, shape, orientation and spatial distribution of θ' precipitates that hinder dislocation slip but there are not multiscale simulations tools that can predict the features of these precipitates during high temperature aging. In this investigation, the evolution and equilibrium morphology of the θ' precipitates in 3 dimensions during high temperature aging is studied by means of a multiscale approach. The lattice parameters and elastic constants of θ' precipitates and of the a-Al matrix were calculated using first principles density functional theory, whereas the interfacial energy between θ' phase and a-Al matrix was determined by means of molecular dynamics. The equilibrium shape and the evolution of θ' precipitates with and without including the presence of dislocations was studied using the phase field method. The simulations indicate the plate-like shape of the θ' precipitates comes about from the competition of the elastic strain energy and the interfacial energy. Moreover, the high aspect ratio of θ' precipitates is induced by the shear strain and interfacial energy anisotropy. It is shown that the stress field of pre-existing dislocation may result in a series of parallel θ' precipitates forming along the dislocation line. Finally, the results of the multiscale simulations in terms of precipitate shape, size and spatial distribution are compared with detailed transmission electron microscopy observations on Al-4 wt. % Cu alloys that were aged at 180ºC for up to 30 hours.

10:00 AM Break

10:30 AM

Linked Heat Treatment and Bending Simulation of Aluminum Tailored Heat Treated Profiles: *Hannes Fröck*[1]; Matthias Graser[2]; Michael Reich[1]; Michael Lechner[2]; Marion Merklein[2]; Olaf Kessler[1]; [1]University of Rostock; [2]Friedrich-Alexander-Universität Erlangen-Nürnberg

Precipitation hardening aluminum alloys enable tailoring of mechanical properties by the dissolution of strength-increasing precipitates during a local short-term heat treatment. Tailored Heat Treated Profiles (THTP) are aluminum extrusion profiles with locally different material properties, specifically optimized for succeeding bending processes. Softened areas need to be generated next to hardened areas to optimize the material flow during the forming process. To determine the optimized layout of softened and hardened areas, a process chain simulation consisting of the simulation of the short-term heat treatment and the subsequent forming process seems purposeful. The numerical modeling of short-term heat treatment requires a coupled computation of thermal and mechanical simulation with particular focus on the evaluation of microstructure and consequently on the change of mechanical properties. The dissolution and precipitation behavior during heating and cooling of aluminum profiles 6060 T4 is investigated using differential scanning calorimetry. Thermo-mechanical analysis is applied for evaluation of the mechanical properties. This behavior should be described in a material model with the software LS DYNA. The heat treatment simulation provides a distribution of mechanical properties along the profile, which is an important input parameter for the following forming simulation. In order to avoid a loss of information between the heat treatment simulation and forming simulation, both linked simulations are performed with the software LS DYNA.

10:50 AM

Numerical Simulation of Meso-micro structure in Ni-based Superalloy during Liquid Metal Cooling Process: *Xuewei Yan*[1]; Wei Li[2]; Lei Yao[2]; Xin Xue[2]; Yanbin Wang[2]; Gang Zhao[2]; Juntao Li[2]; Qingyan Xu[1]; Baicheng Liu[1]; [1]Tsinghua University; [2]Beijing CISRI-GAONA Materials & Technology Co. LTD

Ni-based superalloys are the preferred material to manufacture turbine blades for their high temperature strength, microstructural stability and corrosion resistance. As a new method, liquid-metal cooling (LMC) process is prospective used in manufacturing large-size turbines blades. Unfortunately, there are many casting defects during LMC directional solidification, such as stray grain, freckle, cracking. Moreover, the trial and error method is time and money cost and lead to a long R&D cycle. As a powerful tool, numerical simulation can be used to study LMC directional solidification processes, to predict final microstructures and optimize process parameters. Mathematical models of microstructure nucleation and growth were established based on the cellular automaton-finite difference (CA-FD) method to simulate meso-scale grain and micro dendrite growth behavior and morphology. Simulated and experimental results were compared in this work, and they agreed very well with each other. Meso-scale grain evolution and micro dendritic distribution at a large scale were investigated in detail, and the results indicated that grain numbers reduced with the increase of height of the casting, and stray grain will be relatively easy to produce in the platform. In addition, secondary dendrite arms were very tiny at the bottom of the casting, and they will coarsen as the he height of the cross section increased.

11:10 AM

A Crystal Plasticity (CP) Model for Dynamic Recrystallization (DRX) in Two Phase Titanium Alloys: *Riddhiman Bhattacharya*[1]; Veera Sundararaghavan[1]; John Allison[1]; [1]University of Michigan, Ann Arbor

Titanium (Ti) alloys are attractive candidates for bladed disk (BLISK) manufacturing due to their high specific strength and retention of mechanical properties up to high temperatures (~500 degree C). However, their susceptibility to contamination in the molten state necessitates use of solid state processing methods, such as Linear/Translation Friction Welding (LFW/TFW). In this process, simultaneous action of strain and temperature at or near the weld interface causes Dynamic Recrystallization (DRX), manifested in the form of fine recrystallized beta grains in a two phase (alpha+beta) alloy. The constitutive response of this phenomenon is experimentally studied and input into an advanced Crystal Plasticity (CP) framework. The model is able to capture the softening in stress-strain behavior occurring due to DRX and predict the recrystallization texture. Future work is directed at predicting the recrystallized microstructure based on certain nucleation conditions and mesh refinement criteria.

11:30 AM

Crystal Plasticity Model For Two Phase Ti-6Al-4V Incorporating Microstructural Variability: *Kartik Kapoor*[1]; Ryan Noraas[2]; Vasisht Venkatesh[2]; Michael Sangid[1]; [1]Purdue University; [2]Pratt & Whitney

Dual phase titanium alloys can be designed and processed to exhibit a wide range of properties depending on component requirements. There is a growing need to understand damage mechanisms in two-phase titanium alloys, such as Ti-6Al-4V, due to their widespread use in the aerospace industry. Ti-6Al-4V microstructures consist of an alpha (HCP) phase and a beta (BCC) phase. In this work, a crystal plasticity finite element (CPFE) model that explicitly incorporates both these phases, and hence the anisotropy between them is developed. The finite element microstructural mesh used for the CPFE simulations is created using data obtained from electron backscatter diffraction (EBSD) and backscatter electron (BSE) imaging with the former providing the grain orientation and morphology and the latter giving information on the phases. Utilization of this approach ensures that the finite element mesh truly represents the actualmicrostructure of the material. Further, the CPFE model developed is calibrated over a range of different microstructures, including varying beta volume fractions. Since Ti-6Al-4V components can be manufactured to meet a range of microstructure and property requirements, a robust crystal plasticity model for this alloy should be valid over a range of heat treatment variations and associated microstructures. Finally, the implications of this work looks at linking microstructural features to damage in two-phase titanium alloys.

11:50 AM

CALPHAD Modeling Tools for ICME Applications: *Fan Zhang*[1]; Shuanglin Chen[1]; Weisheng Cao[1]; Chuan Zhang[1]; Jun Zhu[1]; [1]CompuTherm, LLC

Integrated Computational Materials Engineering (ICME) has recently been highlighted as a methodology that can unlock great potential for significant benefits in cost-effective materials and process design. Optimization of alloy chemistry and processing conditions, which is the common practice of materials scientists/engineers working on materials design and improvement, is no longer based on trial-and-error approaches. With the recent advancement of computer science and modern information technology, alloy design process can be greatly accelerated with the aid of computational tools. While the initiative of ICME and MGI has motivated the use and development of modeling tools, the CALPHAD-based modeling tools have been used for alloy design for more than 20 years. The CALPHAD method, which was first developed for the calculation of multi-component complicated phase diagrams, has now been applied to variety fields of materials science and engineering. CALPHAD-based modeling tools have extended their capability from calculating phase stability and thermodynamics of a materials system to simulating precipitation and diffusion kinetics. These modeling tools have been used by ICME practitioners on daily basis to accelerate alloy design and development. In this presentation, we will give a brief introduction on the modeling tools developed at CompuTherm based on the CALPHAD method. Unique features of our modeling tools, such as contour diagrams, high-throughput calculations, will be highlighted. We will then use examples to demonstrate the successful applications of these modeling tools in ICME and MGI.

12:10 PM Lunch on Your Own

Phase Field Modeling - I

Tuesday AM
May 23, 2017

Room: Salon IV
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

8:00 AM

Multiscale Simulation of \945-Mg dendrite growth via 3D Phase Field Modeling and Ab-initio First Principle Calculations: Jinglian Du[1]; Zhipeng Guo[1]; Manhong Yang[1]; *Shoumei Xiong*[1]; [1]Tsinghua University

Based on synchrotron X-ray tomography and electron backscatterd diffraction techniques, recent studies reveal that the \945-Mg dendrite exhibits a morphology of 18 primary branches in 3D, of which six grow along <11-20> on the basal plane, whereas the other twelve along <11-23> on the non-basal plane. To describe this growth behaviour and simulate the morphology of the \945-Mg dendrite in 3D, an anisotropy function based on cubic harmonics was developed and coupled into a 3D phase field model previously developed by the current authors. Results showed that this anisotropy funtion together with the phase field model could perfectly describe the 18-branch dendrite morphology for the magnesium alloys. The growth tendency or orientation selection of the 18-branch morphology was further investigated by performing ab-initio first principle calculations based on the hexagonal symmetry structure. It was showed that those crystallographic planes normal to the preferred growth directions of \945-Mg dendrite were characterized by higher surface energy than these of others, i.e. coinciding with the 18-branch dendritic morphology. Apart from agreement with experiment results and providing great insights in understanding dendrite growth behaviour, such multiscale computing scheme could also be employed as a standard tool for studying general pattern formation behaviours in solidification.

8:20 AM

Macro- and Micro-Simulation and Experiment Study on Microstructure and Mechanical Properties of Squeeze Casting Wheel of Magnesium Alloy: *Shan Shang*[1]; Bin Hu[2]; Zhiqiang Han[1]; Weihua Sun[3]; Alan Luo[3]; [1]Tsinghua University; [2] General Motors China Science Laboratory; [3]The Ohio State University

The macro- and micro-simulation based on a coupled thermo-mechanical simulation method using ANSYS® and phase field modeling with pressure effects were carried out for squeeze casting wheel of AT72 alloy. The mechanical properties at different positions of the wheel and under different pressures were analyzed by the macro- and micro-simulation and experimental results, and the corresponding strengthening mechanism was discussed. Firstly, the mechanical properties in spoke are better than those in rim due to higher integrity associated with more forced feeding including more liquid flow feeding and almost all of the plastic deformation feeding in spoke. Furthermore, the mechanical properties increase with pressure due to the enhanced forced feeding shown by the macro-simulation results and the more developed dendrite arms, finer dendrites and more solutes in dendrites under higher pressure indicated by the micro-simulation and experimental results. As analyzed, the mechanical properties are improved by applied pressure according to the strengthening mechanism, including strengthening associated with high integrity, fine-grain strengthening and solution strengthening.

8:40 AM

Solidification Simulation of Fe-Cr-Ni-Mo-C Duplex Stainless Steel using CALPHAD-coupled Multi-phase-field Model with Finite Interface Dissipation: *Sukeharu Nomoto*[1]; Kazuki Mori[1]; Masahito Segawa[2]; Akinori Yamanaka[2]; [1]ITOCHU Techno-Solutions Corporation; [2]Tokyo University of Agriculture and Technology

A multi-phase-field (MPF) model with finite interface dissipation proposed by Steinbach et al. is applied to simulate dendritic solidification in Fe-Cr-Ni-Mo-C duplex stainless steel. This MPF model does not require the equal diffusion potential assumption and can take into account strong non-equilibrium interfacial condition. We develop the MPF code for coupling with CALPHAD thermodynamic database in order to simulate two-dimensional microstructure evolutions in multi-component alloys by using TQ-interface of Thermo-Calc. MPI parallelization technique is adapted to the program code development to reduce computational elapse time. It is confirmed that the developed MPF code can give highly stabilized calculation in some different initial composition conditions of the continuous casting process. The reliability of the obtained microstructure evolutions will be qualitatively discussed by comparing with the recent experimental observation.

9:00 AM

A Cellular-automata Model for Dynamical Recrystallization with Using the Cell-orientated Grain Boundary Velocities: *Daliya Aflyatunova*[1]; [1]The University of Sheffield

The recrystallization and the grain growth in metals strongly influences on the microstructure and final properties, but it is difficult to study by experimental and statistical methods. Last decade CA technique was successfully applied [1] for recrystallization and grain growth [2] using cellular automata. However the used distance variable which corresponds to the grain boundary velocity was not considered as orientation depended and was the same for all direction of moving grain boundary interface. The current work suggests an extended CA technique which includes into consideration of the grain boundary velocity for each of the neighboring cell, thereby changing switching probability depending on the direction of the grain boundary movement. The results showed that the method is robust and is in agreement with the previously developed models, nevertheless is more physically correct. 1. G. Kugler, R. Turk. Modeling the dynamic recrystallization under multi-stage hot deformation. Acta Materialia, 2004.2. Ye. Vertyagina, M. Mahfouf, and X. Xu. 3d modelling of ferrite and austenite grain coarsening using real-valued cellular automata based on transition function. Journal of Materials Science, 48(16): 5517- 5527, August 2013.

9:20 AM

Effect of Mn Diffusivity on the Austenite-to-ferrite Transformation Behavior in Fe-C-Mn Ternary Alloy: A Multi-phase-field Study: *Takahiko Kohtake*[1]; Akinori Yamanaka[2]; Yoshihiro Suwa[1]; [1]Nippon Steel & Sumitomo Metal Corporation; [2]Tokyo University of Agriculture and Technology

The austenite-to-ferrite (\947-to-\945) transformation in a Fe-C-Mn alloy is one of the important solid-solid phase transformations for steel-making processes. However, because there is a large difference in diffusion coefficient between Mn and C atoms in the alloy, the transformation behavior strongly depends on the chemical composition and temperature. Recently, the multi-phase-field (MPF) method has attracted much attention as a tool for understanding the transformation behavior. However, to the best of the authors' knowledge, few quantitative investigations of the interfacial migration and the diffusion of the alloying elements during the \947-to-\945 transformation by the MPF method have been reported. Therefore, we have investigated the Mn diffusivity's effect on the \947-to-\945 transformation by the one-dimensional MPF simulation coupled with the thermodynamic database based on the CALPHAD method. In this study, in order to further clarify the Mn diffusivity's effect on the transformation kinetics, we perform the MPF simulation of the \947-to-\945 transformation using the various ratio of the Mn diffusion coefficient to that of C from 0 to 1 under the condition of the fixed C diffusion coefficient. The results clarify that when the Mn diffusivity is sufficiently high, Mn atoms are partitioned between \947 and \945 during the transformation. On the other hand, when the Mn diffusivity is low, the \947-to-\945 transformation proceeds without Mn partitioning. Furthermore, it is interestingly found that, for a case of intermediate Mn diffusion coefficient, the \947-to-\945 transformation stagnates after the transformation without Mn partitioning. In this presentation, several factors for this stagnation will be discussed.

9:40 AM

Full Field Simulation of the Recrystallization during Annealing of AZ31 Mg Alloy Taking into Account Plastic Deformation and Twinning: *Alvaro Ridruejo*[1]; Raul Sanchez-Martin[2]; Efim Borukhovich[3]; Reza Darvishi Kamachali[4]; Oleg Shchyglo[4]; Ingo Steinbach[4]; Javier Segurado[1]; Javier LLorca[2]; [1]Technical University of Madrid; [2]Imdea-Materials Institute; [3]KTH Royal Institute of Technology; [4]ICAMS, Ruhr-Universität Bochum

Microstructural optimization of metallic alloys is carried out by means of thermo-mechanical processes. The microstructural changes are controlled by a number of factors that include the details of the initial microstructure and the driving forces and kinetics processes associated with temperature (diffusion, phase transitions) as well as mechanical deformation (elastic strain energy, twinning, etc.). In this work, a full-field approach capable of taking into account these phenomena is presented. In this approach, the phase field model of microstructure evolution is coupled with a dislocation-based crystal plasticity model to account for the mechanical effects. In addition to conventional dislocation glide, the model is able to account for plastic deformation by mechanical twinning, which is simulated as a mechanically-driven solid-state phase transformation. The full field model is used to simulate the effect of prior mechanical deformation on the recrystallization and texture evolution during high temperature annealing of an AZ31 Mg alloy sheet. Our findings suggest that the inhomogeneous distribution of energy stored within the grains after deformation leads to a notable reduction of the initial basal texture during subsequent recrystallization processes. These results are validated by experiments where the texture evolution during annealing of an AZ31 magnesium sheet, previously deformed by in-plane compression, was measured. Finally, it is confirmed that the full field model can be used to simulate the complete sequence of deformation and recrystallization steps during sheet metal manufacturing.

10:00 AM Break

10:30 AM

Using the PRISMS-PF Phase Field Code in an ICME Framework to Examine Precipitates in Mg-Nd Alloys: *Stephen DeWitt*[1]; Shiva Rudraraju[1]; Katsuyo Thornton[1]; Anton Van der Ven[2]; John Allison[1]; [1]University of Michigan - Ann Arbor; [2]University of California - Santa Barbara

We introduce PRISMS-PF, a new, advanced open source phase field modeling code, and its application to simulate precipitate microstructures. PRISMS-PF provides a simple, flexible interface for massively parallel phase field simulations. Leveraging the deal.II finite element library and its matrix-free framework, improved performance over finite difference codes

and traditional finite element codes is demonstrated. Using PRISMS-PF, we investigate precipitate formation in magnesium-rare earth alloys, which have garnered substantial interest as a structural material for automotive and aerospace applications. In one magnesium-rare earth alloy, magnesium-neodymium, recent experimental and first-principles work indicates that the alloy's high strength is due to β''' precipitates. We conducted phase field simulations of these precipitates, examining the morphology of isolated precipitates and the evolution of interacting precipitates, with inputs determined from first-principles calculations. Simulations of isolated precipitates predict the habit plane seen experimentally, (100), but predict that the precipitates are longer in the [010] direction than the [001] direction, in contrast to observations. Systematic variation of the model parameters within the first principles calculation uncertainty indicates that the discrepancy may not be fully explained by uncertainty in the inputs. Simulations of small clusters of precipitates demonstrate that effect of interactions between precipitates also affects their aspect ratio. Accounting for these interactions, parameters within the first-principles uncertainty and consistent with observations are determined and used in a simulation of the nucleation and growth of many β''' precipitates. The predicted volume fraction, number density, and shape distribution as a function of time are compared to experimental observations.

10:50 AM

Phase Field Modeling of Precipitate-Free Zones Around Grain Boundaries: *David Montiel*[1]; Jason Luce[1]; Katsuyo Thornton[1]; [1]University of Michigan

We employ a coupled conserved-nonconserved phase field model with a stochastic nucleation method to simulate the nucleation and subsequent growth of precipitates. This model was implemented into the PRISMS-PF code, an open-source finite element simulation code developed within the PRredictive Integrated Structural Materials Science (PRISMS) Center at the University of Michigan. Using this model, we study the formation of precipitate free zones (PFZs) around grain boundaries during aging. In particular, we focus on the effect of preferential nucleation along a grain boundary and the resulting solute depletion on the formation of the PFZ. In addition, we study the effect of solute diffusivity and of the initial solute supersaturation. We compare our results to experiments including PFZs formed during aging of Mg-RE alloys. We also explore a simplified semi-analytical model that uses the Zener's approximation to describe the solute concentration profile around precipitates.

11:10 AM

Aspects of Microstructure Simulation in ICME: A Virtual Process Chain for Diffusion Brazing of Alloy 24: *Bernd Böttger*[1]; [1]Access eV

Different aspects of microstructure simulation within an ICME setting are discussed with focus on the multiphase-field software MICRESS®. In the first step, microstructure modelling of alloys often needs related input from external sources: Concentration distributions may be read in from experiments, prior simulation runs or other software tools. Particularly in the case of multicomponent systems, thermodynamic data typically is provided by Computational Thermodynamics tools using Calphad databases. During simulation, the microstructure tool must be able to treat phase transformations like melting, solidification or precipitation, different types of diffusion of chemical elements (chemical diffusion, cross diffusion, interface diffusion, infinite diffusion, far-field diffusion, etc.) as well as redistribution of the elements between phases (including solute trapping, para-equilibrium, LENP). Finally, concentration distributions or derived quantities like average compositions or a segregation index can be stored using standardized formats (e.g. HDF5 or VTK) and be handed over to other tools for simulation of subsequent process steps. During the talk, a virtual process chain for diffusion brazing of the Ni-based superalloy M247 is presented which spans the fields between the sub-µ and the macro-scale, between thermodynamic data and properties and between casting and the product life time. The challenges are discussed and the importance of a correct and complete handling of the relevant microstructural quantities in ICME is illustrated.

11:30 AM

Phase-field Modeling of θ' Precipitation Kinetics in W319 Alloys: *Yanzhou Ji*[1]; Bita Ghaffari[2]; Mei Li[2]; Long-Qing Chen[3]; [1]The Pennsylvania State University, University Park; [2]Ford Motor Company; [3]The Pennsylvania State University, University Park

Understanding and predicting the morphology, kinetics and hardening effects of θ' precipitates are critical in improving the mechanical properties of Al-Cu-based alloys through controlling the temperature and duration of any isothermal aging process. In this work, we present a comprehensive phase-field framework for simulating the kinetics of θ' precipitates in W319 alloys, integrating the thermodynamic and diffusion mobility databases of the system, the key anisotropic energy contributions from literature and first-principles calculations, as well as a nucleation model based on the classical nucleation theory. By systematically performing phase-field simulations, we optimize the model parameters to obtain the best possible match to the peak number density, average diameters and volume fractions of θ' precipitates from experimental measurements at 190°C, 230°C and 260°C. With these parameters available, the phase-field simulations can be performed at other aging temperatures. The possible extensions of the current phase-field model for more accurate prediction of the precipitate behaviors in W319 alloys will also be discussed.

11:50 AM

Phase-field Modeling of Cu-Mn-Ni Rich Precipitate Behavior in Reactor Pressure Vessel (RPV) Steel: *Kunok Chang*[1]; Junhyun Kwon[1]; [1]Korea Atomic Energy Research Institute

The late blooming phase (late-stage precipitate) is a limiting factor for the long term operation of the nuclear power plants. The precipitated gamma precipitate cause the late-stage hardening and it reduced the fracture toughness of the RPV steel. The elements consist of the gamma precipitate is Cu, Mn, Ni, Si and other minor alloying elements and we choose three major components (Cu, Mn, Ni) for simplicity. We simulated the behavior of the gamma precipitate (Cu-Mn-Ni rich) in the alpha-Fe matrix. We investigated a role of the dislocation loop on the behavior of the gamma precipitate in the 3-D system. To conduct the simulations, we adopted the thermodynamic database of Fe-Cu-Mn-Ni quaternary system assessed by Koyama et al.. It is demonstrated that the interstitial loop reduce the stability of the gamma precipitate and also it alters the morphology of the precipitate in 3D space.

12:10 PM Lunch on Your Own

Plenary II

Tuesday PM
May 23, 2017

Room: Salon II, III, IV
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

2:00 PM

The Generalized CALPHAD Methodology – The Data Infrastructure of ICME: *John Agren*[1]; [1]Royal Institute of Technology

It has been argued that CALPHAD should be regarded as the first materials genome. Although CALPHAD was initially developed to organize thermochemical and phase equilibrium information it was later extended to handle information on multicomponent diffusion kinetics. In a more general sense CALPHAD should be regarded as the most efficient way of organizing data to make it useful for ICME. Underlying the methodology is the concept of genomic database which consists of the combination a mathematical model and its parameters to represent physical quantities. From a more abstract point of view on may regard a physical quantity as a "vector", the model as the basis and the parameters as coordinates. For example, the CALPHAD method should be extended to represent elastic, thermal, interfacial and mechanical properties. Some recent examples will be discussed.

2:40 PM Invited
Innovations in Experimental Techniques for ICME: *Ji-Cheng Zhao*[1]; [1]The Ohio State University

This talk will summarize recent advancement in experimental techniques for ICME, especially high-throughput experimental techniques. Localized property measurements on composition gradients created in diffusion multiples and other types of gradient-composition samples allow effective collection of composition-dependent properties for the establishment and validation of models for ICME. A newly developed forward-simulation analysis allows us to accurately obtain impurity diffusion coefficients from regular (including pure metal to pure metal) diffusion couple profiles without using isotope tracer experiments. This is especially significant since only a few tracer experiments are performed worldwide each year in recent years, and thus it is impractical to rely on tracer experiments to obtain the thousands of missing impurity diffusion coefficients that are essential for the establishment of reliable diffusion (mobility) databases for ICME. Dual-anneal diffusion multiples (DADMs) enable effective creation of vast diversity of microstructures across wide ranges of compositions as a function of annealing time and temperature, thus providing systematic information on the phase transformation kinetics. Large datasets of composition – precipitation condition – microstructure can now be collected from DADMs for validation of precipitation and microstructure evolution models.

3:20 PM Invited
Robust Information Management System Enabling Multiscale Modeling Within ICME Paradigm: *Steven Arnold*[1]; [1]NASA Glenn Research Center

With the increased emphasis on reducing the cost and time to market of new materials, the need for analytical tools that enable the virtual design and optimization of materials throughout their processing - internal structure - property - performance envelope, along with the capturing and storing of the associated material and model information across its lifecycle, has become critical. This need is also fueled by the demands for higher efficiency in material testing; consistency, quality and traceability of data; product design; engineering analysis; as well as control of access to proprietary or sensitive information. Fortunately, material information management systems and physics-based multiscale modeling methods have kept pace with the growing user demands. Herein, recent efforts to identify best practices and key principles for development of a robust information management system, operational on different length scales, that enables Integrated Computational Materials Engineering (ICME) will be discussed. In particular, the NASA Glenn Research Center efforts towards establishing such a system (for coupling test data and simulation data along with associated pedigree for both monolithic and composite materials) utilizing Granta MI® and NASA GRC's Integrated multiscale Micromechanics Analysis Code (ImMAC) software toolset will be highlighted. These tools, and this type of linkage, are foundational to realizing the full potential of ICME, in which materials processing, microstructure, properties, and performance are coupled to enable application-driven design and optimization of materials and structures

4:00 PM Break

4:20 PM Vendor Showcase - Software Solutions

Plenary III

Wednesday AM
May 24, 2017

Room: Salon II, III, IV
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

8:00 AM Invited
ICME Guided Cast Aluminum and Steel Alloys Development in Automotive Applications: *Mei Li*[1]; [1]Ford Motor Company

To improve the fuel economy and reduce the automobile emissions, high-performance engines and exhaust systems are imperative which require new advanced materials to be able to operate at higher temperatures. The recent advanced engines increase the maximum engine operating temperature from approximately 170°C to well above 200°C, and exhaust components surface temperature beyond 1000°C. The increase in the operational temperatures requires new materials with optimized properties in terms of tensile, fatigue and thermos-mechanical fatigue strength. This talk will present two examples of the important role that ICME plays in accelerating the development of new cast aluminum and Nb-bearing austenitic heat-resistant cast steel alloys, the design and optimization of the performance of the components at Ford, as well as the gaps in meeting the challenging requirements in ICME approach.

8:40 AM Invited
Uncertainty Management and Decision Making in the ICME Process Chain: *Jitesh Panchal*[1]; [1]Purdue University

The management of uncertainty is well recognized as one of the crucial activities in the ICME process. Uncertainty management is broader than uncertainty quantification in modeling and simulation. It involves a number of decisions such as choosing which model to sample from, deciding how much experimental data to gather, deciding whether to refine a model or not, choosing the level of model fidelity, deciding a model validation strategy, deciding whether to reuse existing models or to develop new customized models, deciding which multiscale models to integrate, and deciding to compose models at different scales. Such decisions are further complicated in the presence of human decision makers, multiple teams, and organizational boundaries. The focus in this talk will be on (i) the need for rigorous techniques for making consistent uncertainty management decisions within ICME, (ii) existing decision making frameworks that can be used to address the need, and (iii) the research challenges involved in implementing such frameworks within realistic industrial settings.

9:20 AM Invited
The Materials Project for Accelerated Design of Energy Materials: *Muratahan Aykol*[1]; [1]Lawrence Berkeley National Laboratory

The Materials Project (http://www.materialsproject.org) leverages the exponentially growing computational power of the information age for materials design, with the goal of accelerating the materials development and discovery through advanced scientific computing and innovative design methods. Since its launch in 2011, Materials Project has computed more than 67,000 inorganic compounds using high-throughput density functional theory. A large number of materials properties such as the crystal structure, X-ray diffraction pattern, band structure, battery electrode properties, elastic tensors, stability, reaction energies and more, can be freely accessed and queried through the web interface of Materials Project or its application programming interface (API). In this talk, we will highlight the materials design tools and the data infrastructure that emerged over the years of efforts in applying a materials genomic approach in materials design, and present examples of how the data we produced can be leveraged to design novel energy materials. These examples include novel electrodes and electrolytes in energy storage and production, along with dissemination of phase stability, solid-aqueous stability, elastic properties and electronic structure information across structure and chemical space.

10:00 AM Break

ICME Design Tools and Application - I

Wednesday AM
May 24, 2017

Room: Salon I
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

10:30 AM
OOF: Flexible Finite Element Modeling for Materials Science: *Andrew Reid*[1]; Stephen Langer[1]; Shahriyar Keshavarz[2]; [1]NIST; [2]Theiss Research

The ability to flexibly and rapidly assess the global behavior of various possibly complex model microstructures, and examine variations in both the structure and the component constitutive properties, is a powerful capability for computational materials modelers. The Object-Oriented Finite Element (OOF) software meets this need by providing a mechanism for users to create high-quality finite-element meshes from 2D or 3D microstructural image data, add constitutive rules for the component phases, and perform virtual experiments on these real microstructures. This allows materials scientists who are not experts

in computational methods to rapidly explore structure-property relationships, including assessing effective properties of microstructures, and examining the system under load to investigate the detailed behavior of the system with full spatial resolultion, allowing for an understanding of how the system's response to loads is distributed. The OOF team at the National Institute of Standards and Technology has been working on advanced meshing tools for 3D, the incorporation of crystal plasticity into the OOF system's solid-mechanics suite, and better integration with other 3D data management tools and systems.

10:50 AM

Efficient Global Optimization to Close ICME Loop: Anjana Talapatra[1]; *Thien Duong*[1]; Raymundo Arroyave[1]; [1]Texas A&M University

The implementation of ICME for materials design and discovery requires one important component: an on-the-fly process optimization to close the ICME design/discovery loop. Such an optimization would effectively guide the computational design/discovery process towards its goals under certain engineering constraints. In the current work, we propose the usage of efficient global optimization (EGO) as an effective on-the-fly materials discovery framework within ICME. EGO was initially proposed by D.R. Jones et al. in 1998 for the optimal sequential design of experiments under the assumption that experiments are costly functions that need to be evaluated. In the context of (global) optimization, EGO and its variants is widely used due to the fact that it minimizes the number of function evaluations that need to be carried out in order to optimize the (potentially) multi-dimensional function-to-be-optimized. The proposed framework is based on stochastic regression (Gaussian Processes) and uses expected-improvement as a metric of optimality that balances exploration and exploitation of the design space. The inspiration for this optimization in ICME stems from a recent study on the practical aspect of the optimization of the computer-driven materials discovery process. The current demonstration of EGO and its advantages is carried out in a simple ICME framework integrating first-principle calculations with the optimization itself. The goals of the optimization are to maximize (1) bulk modulus and (2) ductility of MAX phases - a special class of laminated materials that exhibits a merit set of properties combining those of metals and ceramics.

11:10 AM

MUESLI: A Material UnivErSal LIbrary: *Ignacio Romero*[1]; Daniel del Pozo[1]; Daniel Rodríguez Galán[1]; David Portillo[2]; Eva Andrés[1]; Javier Segurado[1]; [1]IMDEA Materials Institute; [2]Technical University of Madrid

Simulation codes in Computational Mechanics employ libraries of materials that model their constitutive response. At the same time, many researchers and code developers in this discipline continue to implement their own advanced material models. However, to the best of the authors' knowledge, there is no way to access this body of knowledge and accumulated experience since computer implementations of material models are not shared. Muesli, a Material UnivErSal LIbrary, is an open source library created to alleviate this situation, simplifying the development and implementation of material models, and their interface with larger research and commercial computational codes. Muesli includes the basic, most commonly used material models in Computational Mechanics. Currently, it contains constitutive models for small strain and finite strain solid, fluid and thermal materials and coupled models. The library has been designed with the following features: * Clarity: Muesli has been developed using the compact notation of C++, whose operator overloading capacity makes the implementation of material models as natural as possible. * Extensibility: Muesli defines a clear hierarchy of material class that makes relatively simple to extend current capabilities. * Reliability: Muesli has automatic checking capabilities to verify the consistency (and up to certain extent the correctness) of the material models. * Plug-ability: Muesli 1.0, provides interfaces that connect the library to two widely employed commercial simulation codes: Abaqus/standard and LS-DYNA.* Freely available: Muesli is distributed to the material science and computational mechanics community under GPL 3.0 license at http://www.materials.imdea.org/Muesli.

11:30 AM

Polymer and Composite Simulation at nanoHUB.org: *Benjamin Haley*[1]; Lorena Alzate Vargas[1]; Chunyu Li[1]; Alejandro Strachan[1]; [1]Purdue University

Amorphous polymers and composites are critical engineering materials with applications ranging from structural components in aircraft and automobiles to packaging in electronics. Predictive atomic-level simulations of these materials are very important 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 polymers and composites and make them widely available for cloud computing via NSF's nanoHUB and freely distributed via Github. The framework under development consists ofthree 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, molecular structures, with predicted and experimental properties. connected to the simulation tools, hosted on nanoHUB iv) connections to external databases of structures and forcefields, outside nanoHUB, like OpenKIM.

11:50 AM

A Constraint Satisfaction Problem Approach to High-Entropy Alloy Design: *Anas Abu-Odeh*[1]; Nayan Chaudhary[1]; Sean Gibbons[2]; Edgar Galvan[1]; Tanner Kirk[1]; Raymundo Arroyave[1]; Richard Malak[1]; [1]Texas A&M University; [2]Air Force Research Laboratory

High-entropy alloys (HEAs) are multi-principal element alloys at near-equiatomic concentrations that can have superior properties such as high irradiation resistance, high fatigue resistance, and high temperature usage, compared to conventional alloys. This gives HEAs potential application to industries such as nuclear, aerospace, medical, and electronic. However, the design and discovery of HEAs has been largely limited to trial and error methods, therefore only a fraction of the possibilities have been produced. A computational alloy design methodology called the Constraint Satisfaction Problem (CSP) approach is proposed to accelerate HEA design and discovery. This approach consists of three major steps: mapping design requirements into mathematical constraints and using computational thermodynamic calculations to implement them, sampling, using genetic algorithms, the HEA space of composition and temperature within the constraints to search for solutions, and describing the final solution space using machine learning methods. Ultimately, the CSP approach enables the identification of all regions in composition space that satisfy material design requirements. A Thermo-Calc database was verified against experimental data in order to implement phase stability calculations. With kinetic considerations, 70.8% of the 216 evaluated alloys showed good agreement between experiments and calculations using the database. This database was used to map out single-phase solid solution regions for the known CoCrFeMnNi HEA and all of its subsequent near-equiatomic quaternary and ternary systems. The results demonstrate the CSP's capability to search HEA thermodynamic space and to accelerate HEA design and discovery.

12:10 PM

Design of Light Weight High-Entropy Alloys: Modeling and Experiments: *Michael Gao*[1]; Rui Feng[2]; Jeffrey Hawk[1]; Paul Jablonski[1]; Chan Ho Lee[2]; Peiyong Chen[3]; David Alman[1]; Peter Liaw[2]; [1]National Energy Technology Lab; [2]University of Tennessee; [3]CompuTherm LLC

Developing high-performance light-weight alloys has been a great challenge in academia and industries due to the difficulty in balancing various properties including strength, ductility, oxidation resistance, and density. In the present study, we have applied the concept of high entropy alloys to the design of new light-weight high-entropy alloys that comprise of main constituent elements Al, Cr, Fe, Mn, Nb, Ti, and V. The alloys are mainly designed using CALPHAD method. First-principles density functional theory calculations, Molecular Dynamics simulations, and Monte Carlo simulations are carried out to predict the structural, thermodynamic, electronic, vibrational, and elastic properties. Guided by the computational predictions, experimental efforts have been carried out in alloy fabrication, heat treatment, microstructure characterization using X-ray diffraction and scanning/transmission electron microscopy, and mechanical property characterization such as hardness, compression and tension tests.

12:30 PM Lunch on Your Own

Integration Framework and Usage - IIA

Wednesday AM
May 24, 2017

Room: Salon II, III
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

10:30 AM

Improving Manufacturing Quality Using Integrated Computational Materials Engineering: *Dana Frankel*[1]; Nicholas Hatcher[1]; David Snyder[1]; Jason Sebastian[1]; Gregory Olson[1]; Gregory Vernon[2]; Wesley Everhart[2]; Lance Carroll[2]; [1]QuesTek Innovations LLC; [2]Honeywell Federal Manufacturing & Technologies

The prediction of materials properties and their variation within a specification or design space is key in ensuring reliable production uniformity. To capture the complex mechanisms that underpin materials' performance, processing-structure-properties links are established using a "systems design" approach. QuesTek has previously utilized multi-scale ICME modeling methodologies and tools (e.g., CALPHAD thermodynamic and kinetic databases, solidification models, strength models, etc.) and advanced characterization techniques to design advanced materials with improved performance. This work focuses on building an ICME infrastructure to predictively model properties of critical materials for energy and defense applications by optimizing existing materials, performing calculations to quantify uncertainty in material properties, and defining target specification ranges and processing parameters necessary to ensure design allowables. Starting with austenitic stainless steels (SS304L) and moving to soft magnetic alloys (Hiperco 50), metal powders for additive manufacturing (AlSi10Mg and Ti-6Al-4V), and glass-ceramic-to-metal seals (Elan/Paliney), we show how these ICME techniques can be used to optimize the manufacturing process of these materials. These efforts provide pathways to novel, fully optimized alloys and production processes using the Accelerated Insertion of Materials (AIM) methodology within ICME. The AIM method will be used for probabilistic properties prediction from material and process variables (e.g., chemistry and processing route) to enable rapid and cost-efficient process optimization. The Department of Energy's Kansas City National Security Campus is operated and managed by Honeywell Federal Manufacturing & Technologies, LLC under contract number DE-NA0002839.

10:50 AM

Creating an Integrated Collaborative Environment for Materials Research: *Matthew Jacobsen*[1]; Mark Benedict[2]; Bryon Foster[2]; Charles Ward[2]; [1]USAF/AFRL; [2]Air Force Research Laboratory

The Integrated Collaborative Environment (ICE) is an emerging ICME cyberinfrastructure that provides a web-based federated software architecture supporting group and project spaces within which researchers can easily organize, share, and collaborate on the results of their experimental and computational efforts. It seamlessly connects researchers with experimental and computational resources for easy generation, collection, and storage of digital data to provide instant access to results with no intermediate transfers. It contains a robust Application Programming Interface (API) for federating any number of applications and repositories in a secure, efficient, and scalable manner. Persistent identifiers, extensive metadata, and object models are used to ensure historical research data are discoverable, interpretable, and reusable. The architecture is designed to be modular and agile for rapid deployment and expansion across disparate organizations. It comprises a number of open-source, commercial, and non-commercial software packages that provide the specific functionality needed to meet the large number of system requirements. The authors will provide an overview of the successful launch of functionalities such as digital workflow management, equipment integration, and object modeling. Additionally, a showcase of emerging developments in Internet of Things (IoT) technology, virtualization for modeling and simulation execution and tracking, and a communal marketplace for the exchange of tools, scripts, and applications will be provided. Finally, a plan for addressing the recent explosion of potential collaborative use cases between ICME organizations will be examined.

11:10 AM Invited

The PRISMS Framework:

An Integrated Predictive Multi-Scale ICME Capability for the Global Materials Community: *John Allison*[1]; [1]The University of Michigan

The Center for PRedictive Integrated Structural Materials Science (PRISMS) is a major Materials Genome Initiative effort creating a unique scientific framework for accelerated predictive materials science. We envision that the PRISMS Framework will enable the rapid insertion of the latest scientific knowledge into next generation ICME tools. There are three key elements of this framework. This first is a suite of high performance, open-source integrated multi-scale computational tools for predicting microstructural evolution and mechanical behavior of structural metals. The second is The Materials Commons, a knowledge repository and virtual collaboration space for curating, archiving and disseminating information from experiments and computations. The third element of the PRISMS framework is set of integrated scientific "Use Cases" in which these computational methods are tightly linked with advanced experimental methods to demonstrate the ability of the PRISMS framework for improving our predictive understanding of magnesium alloys, in particular precipitate evolution and the influence of microstructure on monotonic and cyclic mechanical behavior. This talk will review the Center's progress, plans and opportunities for collaboration.

11:30 AM

The Materials Commons: A Collaboration Platform and Information Repository for the Global Materials Community: *Glenn Tarcea*[1]; Brian Puchala[1]; H. Jagadish[1]; Margaret Hedstrom[1]; Emmanuelle Marquis[1]; John Allison[1]; [1]University of Michigan

Accelerating the pace of materials discovery and development requires new approaches and means of collaborating and sharing information. To address this need, we are developing the Materials Commons, a collaboration platform and information repository for use by the structural materials community. The Materials Commons has been designed to be a continuous, seamless part of the scientific workflow process. Researchers 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. Using a rich and powerful data model and provenance, the Materials Commons can reveal processing-structure-property relationships and enable 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, as well as for searching and sharing data. This paper provides an overview of the Materials Commons. Concepts are also outlined for integrating the Materials Commons with the broader Materials Information Infrastructure that is evolving to support the Materials Genome Initiative.

11:50 AM

Towards Bridging the Data Exchange Gap Between Atomistic Simulation and Larger Scale Models: *David Reith*[1]; Mikael Christensen[1]; Walter Wolf[1]; Erich Wimmer[1]; Georg Schmitz[2]; [1]Materials Design; [2]MICRESS group at Access e.V.

The origin of most materials properties is rooted in the atomic scale. A detailed microscopic understanding of the physics and chemistry is thus mandatory for successful computational materials engineering. The MedeA computational environment provides a very efficient tool to perform atomistic simulations to predict materials properties from the fundamental interactions effective at the nanoscale. Nevertheless, many interactions and processes occur at much larger time and length scales, that need to be studied with microscale and macroscale models, as exemplified by the multiphase field tool MICRESS. The predictive power of these larger scale models can be greatly increased by augmenting them with atomistic simulation data. The notion of per phase-properties including their anisotropies provides e.g. the key for the determination of effective properties of multiphase materials. The key goal of the present work is to demonstrate the interoperability between atomistic and larger scale models using a data centric approach, in which the "interface" is provided by means of a standardized data structure based on the hierarchical data format HDF5. The example HDF5 file created in Ref. [1], describing a three phase Al-Cu microstructure, is taken and extended to include atomistic simulation data of the Al-Cu phases, e.g., heats of formation, elastic properties, interfacial energies etc. This is pursued with

special attention on using metadata to increase transparency and reproducibility of the data provided by the atomistic simulation tool MedeA. [1] Georg Schmitz et al., Sci. Technol. Adv. Mater. 17 (2016) 411

12:10 PM

A Flowchart Scheme for Information Retrieval in ICME settings: *Georg J. Schmitz*[1]; [1]Micress/Aachen

Interoperability between models implies the need for a flow of information and also a timing of different operations. Getting such workflows well-defined, operational and extendable needs some structural considerations. An instructive approach is seen in decision making workflows, where flowchart tools are used to control and steer the workflow. The proposed flowchart scenario is based on the description of a system state and its evolution by phenomena occurring at all scales. The system state defines the properties which can be extracted from the system state information. A generic classification of models is proposed being based on the functionality of the physics equation like (i) Evolution equations, (ii) Property equations, (iii) Balance equations, and (iv) Conservation equations. Evolution models –EVOLVERS - turn the actual state into a new state at a later time and accordingly change the state. Tools extracting desired properties from as state are called EXTRACTORS. They do not alter the state and thus can operate in parallel to EVOLVERS. Balance type equations allow describing aspects of the equilibrium state thus providing criteria e.g. for the termination of EVOLVERS. Above tools have to be complemented by INPUT/OUTPUT and especially by DECISION tools allowing steering the workflow. The presentation will provide first examples of flowcharts being applied to information retrieval in ICME settings. The research leading to these results has been performed within the ICMEg project and has received funding from the European Union Seventh Framework Programme (FP7/2007-2011] under grant agreement n° 6067114 .

12:30 PM Lunch on Your Own

ICME Success Stories and Applications - I

Wednesday AM
May 24, 2017

Room: Salon IV
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

10:30 AM

Ferrium M54 – ICME Development from Genome to Flight: *Jason Sebastian*[1]; Greg Olson[2]; [1]QuesTek Innovations; [2]QuesTek & Northwestern University

QuesTek Innovations, a leader in the field of Integrated Computational Materials Engineering (ICME), will present a "success story" overview of the development of their new ultra-high strength, high performance structural steel, Ferrium® M54™. The development of this alloy was sponsored under a U.S. Navy-funded Small Business Innovation Research (SBIR) program with the goal of developing a cost competitive, drop-in replacement for AerMet®100 aerospace alloy. A variety of ICME- and "Accelerated Insertion of Materials (AIM)"-type computational models were employed during the design and development of M54, and highlights will be presented. M54's overall development progressed from a clean sheet design in 2007 to a precise chemical composition in less than one year, and the first 10-ton VIM/VAR ingot was produced the following year. An Aerospace Material Specification (AMS 6516) was issued two years later, and inclusion in the MMPDS handbook for A- and B- basis design minima was approved in December 2013. QuesTek coordinated the production and qualification of hook shank components made from M54 that were successfully flight tested in December 2014. Highlights will be presented from a recent (August 2016) National Institute of Standards and Technology-funded case study (carried out by Nexight Group and Energetics Incorporated) detailing overall timeline of the successful development of M54 and its application to U.S. Navy hook shanks. Results and data for M54 will be presented from throughout the alloy development process, with a focus on the properties that distinguish it from legacy materials. Highlights of recent M54 application and commercialization activities will also be presented.

10:50 AM

CASM: Design Principles, Recent Progress, and Collaborative Opportunities: *Brian Puchala*[1]; John Thomas[2]; Anton Van der Ven[2]; [1]University of Michigan, Ann Arbor; [2]University of California, Santa Barbara

Cluster expansion effective Hamiltonians provide a rigorous link between very accurate atomistic scale first principles calculations and very efficient meso- and macro-scale continuum methods for describing materials thermodynamics and kinetics. To implement these methods we are developing the open source software package CASM (github.com/prisms-center/CASMcode). CASM automates the process for 1) formulating effective Hamiltonians based on the symmetry of the crystal system and relevant atomistic degrees of freedom, 2) parameterizing effective Hamiltonian coefficients from first principles calculations, and 3) calculating finite temperature thermodynamic and kinetic properties, such as composition and strain-dependent free energies and diffusion coefficients, using Monte Carlo methods. In this talk I will present CASM design principles and concepts, recent progress, and the direction of its near-term development. I will highlight opportunities for collaborative development of new features and integration with methods at lower and higher length scales. Developed with support from the Center for PRedictive Structural Materials Science (PRISMS) at the University of Michigan, CASM provides an essential component for integrated computational materials engineering.

11:10 AM

Materials Informatics and Big Data: Realization of 4th Paradigm of Science in Materials Science: *Ankit Agrawal*[1]; Alok Choudhary[1]; [1]Northwestern University

In this age of "big data", large-scale experimental and simulation data is increasingly becoming available in all fields of science, and materials science is no exception to it. Our ability to collect and store this data has greatly surpassed our capability to analyze it, underscoring the emergence of the fourth paradigm of science, which is data-driven discovery. The need to use of advanced data science approaches in materials science is also recognized by the Materials Genome Initiative (MGI), further promoting the emerging field of materials informatics. In this talk, I would present some of our recent works employing state-of-the-art data analytics for exploring processing-structure-property-performance (PSPP) linkages in materials, both in terms of forward models (e.g. predicting property for a given material) and inverse models (e.g. discovering materials that possess a desired property). Some examples include developing models for predicting fatigue strength of steel alloys, data-driven discovery of stable compounds, and microstructure optimization of a magnetostrictive Fe-Ga alloy. I will also demonstrate some online web-tools we have developed that deploy machine learning models to predict materials properties.Such data-driven analytics can significantly accelerate prediction of material properties, which in turn can accelerate the optimization process and thus help realize the dream of rational materials design. The increasingly availability of materials databases along with groundbreaking advances in data science approaches offers lot of promise to successfully realize the goals of MGI, and aid in the discovery, design, and deployment of next-generation materials.

11:30 AM

HPC4Manufacturing Program: A National Laboratory - Industry Partnership in High Performance Computational Simulations for Energy Efficiency: *Robin Miles*[1]; Peg Folta[1]; Jeff Roberts[1]; [1]Lawrence Livermore National Laboratory

The HPC4Manufacture program is a new EERE-sponsored program with the aims of introducing industry to High Performance Computing for advanced science and engineering simulations, transferring advanced simulation techniques developed at the National Laboratories to industry and reducing industrial energy usage. The three partner national laboratories have been working with a variety of large and small companies in a variety of energy intensive industries to improve manufacturing processes and enhance product design. Examples include optimizing steel-making furnaces to reduce energy and coke usage and advanced CFD modeling of turbines used for aerospace and energy generation. Many companies are interested in advanced simulation as a way to reduce costs associated with product/or and process testing. An overview of the program will presented and example projects discussed.

11:50 AM

ICME in Design of Hard Materials and Substitution of Critical Raw Materials: *Anssi Laukkanen*[1]; Tatu Pinomaa[1]; Tom Andersson[1]; Matti Lindroos[1]; Tomi Suhonen[1]; Kenneth Holmberg[1]; [1]VTT

The Process-Structure-Properties-Performance (PSPP) paradigm is emerging as one of the cornerstones of implementing integrated computational materials engineering (ICME) for materials R&D needs, such as discovery and development of novel material solutions, optimization and tailoring of product specific materials, and overall troubleshooting materials affiliated problems. We present a case study employing an in-house multiscale materials modeling toolset in design of WC-Co hard materials and TiC-Ni critical raw material substitutes. The approach merges phase field and kinetics modeling of material processing to imaging based modeling of material nano-microstructure to establish causal material properties and performance under typical application environments. Computation driven material design aspects are addressed by an informatics solution incorporating evolutionary computing and machine learning. The results demonstrate how ICME can be applied in designing novel composite materials and finding substitute candidates.

12:10 PM

Developing Cemented Carbides through ICME: *Yong Du*[1]; Yingbiao Peng[2]; Peng Zhou[3]; Weibin Zhanga[1]; Cong Zhang[1]; Na Li[1]; Chong Chen[1]; Yaru Wang[1]; Yafei Pan[1]; Kaiming Cheng[1]; Haixia Tain[1]; Han Li[1]; Li Chen[1]; Wen Xie[4]; Jianzhan Long[4]; Guanghua Wen[4]; Shequan Wang[4]; Zhongjian Zhang[4]; Tao Xu[4]; [1]Central South University; [2]Hunan University of Technology; [3]Hunan University of Science and Technology; [4]Zhuzhou Cemented Carbide Cutting Tools Inc

The ICME (Integrated Computational Materials Engineering) for cemented carbides aims to combine key experiments with multi-scale simulations from nano(10-10~10-8 m) to micro(10-6~10-4 m) to meso(10-4~10-2 m) and to macro(10-2~10 m) during the whole R&D process of cemented carbides. Based on ICME, the framework for R&D of cemented carbides, involving end-user demand, product design and industrial application, is established. In this work, a description to our established thermodynamic and thermophysical (diffusion coefficient, interfacial energy, and thermal conductivity and so on) databases is presented, followed by simulation of microstructure evolution during sintering of cemented carbides by means of phase field method. Work is also done to investigate the correlation between microstructure and mechanical properties (crack, stress distribution, and coupled temp-displacement) by using phase field and finite element methods. The proposed ICME for cemented carbides is used to develop a few new cemented carbides (including gradient cemented carbides, cellular cemented carbides, and ultra-fine cemented carbides), which have found industry applications.

12:30 PM Lunch on Your Own

ICME Design Tools and Application - II

Wednesday PM
May 24, 2017

Room: Salon I
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

2:00 PM Invited

Interoperability and Simulation Platforms for ICME: *Adham Hashibon*[1]; [1]Fraunhofer IWM

The success of ICME hinges on the availability of capable computational modelling tools that can be readily integrated in complex workflows describing complex materials behaviour on multiple scales. Open Simulation Platforms (OSP) offer means to link and couple various existing and well established simulation tools as well as post and pre-processing tools into one computational environment that cover all models and scales. The underlying framework should provide a layer of interoperability to facilitate efficient linking and coupling between existing tools each having its own data structures and semantics. In this talk, a metadata schema allowing both semantic and syntactic interoperability layers between different computational and experimental tools and methods will be presented. The metadata schema as implemented within the SimPhoNy Open Simulation environment will be demonstrated along with various applications linking atomistic and continuum models. An extension of the schema to describe experimental data as well as process parameters will also be demonstrated.

2:30 PM

ICME-based Alloy Design for New Lightweight Titanium Alloys: *Zhi Liang*[1]; Jiashi Miao[1]; Alan Luo[1]; James Williams[1]; Anil Sachdev[2]; [1]The Ohio State University; [2]General Motors

Integrated Computational Materials Engineering (ICME) is an important approach used in materials design and process development. In this paper, computational phase equilibrium based on CALPHAD (CALculation of PHAse Diagrams) methodology has been used to design new cost-effective titanium alloys. The Ti-Al-Fe-B-C system was selected as an example to illustrate the role of ICME in the alloy design process. Several Ti-rich alloys in Ti-Al-Fe-B-C system were investigated for phase equilibria and transformation paths during solidification and heat treatment. This paper presents an ongoing effort to broaden the application of the ICME approach in accelerating the design of multi-component titanium alloys for structural applications.

2:50 PM

First Principle Investigation of Interfacial Energetics Between Ag Alloys and Amorphous SiO2: *Mingfei Zhang*[1]; Liang Qi[1]; [1]University of Michigan-Ann Arbor

Alloy/amorphous interfaces are among most important heterogeneous structures because various thin films are present in optical coatings, semiconductor devices and catalysts. From the thermodynamic point of view, the most critical property to determine thin film quality lies in the adhesion energy of interface. To obtain alloy/amorphous interfaces with strong adhesion requires detailed investigations at atomistic scale. However, interface study of alloy/amorphous at atomistic scale is challenging. To study this system, we need to be mindful of two major problems: to obtain the correct atomistic structures at the interface and to generate the proper alloy distribution near the interface. In order to solve the first problem, we combine long-time classical MD and ab-initio MD to get the amorphous SiO2 structures and SiO2-Ag interfacial structures. For the second problem, we use Special Quasi-random Structure (SQS) to generate multiple random alloy distribution near the interface and obtain the average effect, in which way these configurations can be good representations of the statistical ensemble. By combing these two methods, we examine the alloying effects (10 at% with each of the 3d transition metals as the alloy element) on the adhesion energy between Ag and amorphous SiO2, and discuss their trends based on electronic structures.

3:10 PM

High-throughput Computational Design of Heteroepitaxial Metals with Novel Properties: *Yang Wang*[1]; Samuel Reeve[1]; Alejandro Strachan[1]; [1]Purdue University

Underlying any materials response to mechanical deformation or temperature change is its free energy landscape, the free energy as a function of lattice parameter (or other relevant reaction coordinate). We demonstrate an approach for designing metamaterials via heteroepitaxial integration of metals based on the features of their free energy landscapes. With appropriate combinations of metals unprecedented properties are made possible: ultra-low stiffness, ultra-low thermal expansion and martensitic behavior from non-martensitic components. We conduct density functional theory (DFT) simulations and use the PRISM Uncertainty Quantification (PUQ) software to establish a library of free energy landscapes for a wide range of face-centered cubic (FCC) and body-centered cubic (BCC) metals. Combinatorial searches of these landscapes for the desirable properties above point to potentially interesting superlattice systems. We show that the properties of direct DFT simulations for heteroepitaxial superlattices along the Bain path agree with analytical combination of the free energy landscape of individual constituents. This method of free energy landscape engineering enables efficient direction of further computational and experimental studies of epitaxially integrated metals with novel properties.

3:30 PM Break

3:50 PM

ICME-based Process and Alloy Design for Vacuum Carburized Steel Components with High Potential of Reduced Distortion: Hamidreza Farivar[1]; Gerald Rothenbucher[2]; *Ulrich Prahl*[1]; Ralph Bernhardt[2]; [1]Steel Institute, RWTH Aachen University; [2]Simufact Engineering GmbH

Carburized steel components are usually quenched from a hardening temperature, which lies in a complete austenitic phase, to room temperature. This leads to a microstructure comprised of mostly martensite plus bainite giving rise to unwanted heat-treatment-induced distortion. However, having a soft phase of ferrite dispersed throughout the microstructure can be quite effective in this regard. This is attributed to the capability of ferrite in accommodating the plasticity resulted from austenite-to-martensite transformation expansion. In the context of this work, it is demonstrated that how a proper selection of chemical compositions and a hardening temperature can greatly suppress the associated distortion. Hence, in order to systematically design a new steel alloy which fits to the above mentioned conditions, an ICME-based methodology has been employed. Thus, a series of calculations have been carried out by means of the well-known thermodynamic-based software Thermo-Calc® and the scripting language of Python. The austenite to ferrite phase transformation kinetics is also captured by the software DICTRA® generating a virtual TTT (Time-Temperature-Transformation) diagram which is subsequently utilized for further finite element simulations in the software Simufact.forming®. The carburizing process, the following phase transformations and the effect of the developed microstructure on the final distortion are simulated in macro-scale through Simufact.forming. The finite-element-based results of the Simufact. forming have in turn been enhanced by the results of the above-mentioned thermodynamic-based computational tools. At a later stage the simulation outcomes are experimentally validated by employing Navy C-Ring specimens.

4:10 PM

ICME for Product Development: Role of Multi-scale Models of Casting in Optimizing Product Quality and Cost: Ashwani Pandey[1]; Tushar Telmasre[1]; *Amarendra Singh*[1]; [1]IIT Kanpur

The properties and quality of any cast products are defined in terms of its structure, micro- and macro, and defects such as micro- and macro-segregation of solute and impurities, inclusions, micro- and macro-porosity, cracks, etc. The structure and defects, in turn, are dependent on the process parameters of incoming liquid metal such as temperature, composition, and the level of impurities and the process and design parameters of casting. Downstream operations as well as final product quality are majorly influenced by the quality of the cast product. Defect minimization in casting is therefore of great importance. Also, there is a cost associated with defect minimization. In the context of ICME, defect minimization is closely related to defect quantification with the help of predictive models of casting. Though individual aspects of various phenomena of casting are well researched, the focus has seldom been from product perspective. In this paper, we present some of the recent work on the role of multi-scale model of casting in defect quantification and show how the predictive capability of the model is essential in linking the upstream and downstream operations and thereby meeting the objectives of ICME based product development.

4:30 PM

A Systems Approach for Modeling the Dynamic Thermomechanical Response of Carbon Steels: *Shengyen Li*[1]; Steven Mates[1]; Mark Stoudt[1]; Carelyn Campbell[1]; Greta Lindwall[1]; Sindhura Gangireddy[1]; [1]National Institute of Standards and Technology

In manufacturing processes, workpiece materials are subjected to rapid heating, high loading rates and large plastic strains. Depending on the temperatures involved, the phase transformations that can occur may significantly affect the mechanical behavior, for example when pearlite transforms to austenite in carbon steel. To capture these processing-structure-properties relations, we have a developed a workflow platform to integrate data collection, model simulation, and software applications. Within this platform, microstructure information, thermomechanical data, and mechanical measurements are all easily entered in the Materials Data Curation System (MDCS). This allows the data to be easily transformed and used with other software. For example, simple scripts allow all the SEM micrographs to be access and analyzed by image processing software to determine phase fraction values, which are then stored in the MDCS for later use with other models. CALPHAD-based phase equilibrium calculations are integrated with precipitation and phase transformation models. These results are then integrated with the experimental data and constitutive models to predict time-dependent plastic deformation under rapid heating and loading. This flexible design framework enables the integration of experimental data and composition-dependent models to rapidly develop processing-structure-property relations.

4:50 PM

Thermocalc Tooling Aided Alloy Design and Processing Optimization for Stainless Steels: *laizhu Jiang*[1]; Binghe xiang[1]; [1]Tsingtuo Group

Both the product development and the processing optimization for stainless steels have been extensively carried out through Thermocalc Tooling simulation. Two very important examples were presented here. One is regarding alloy design and hot working temperature assessment for two super duplex stainless steel grads, namely 2507 and 2760. The alloy design is very well balanced among PREN(pitting corrosion resistance=Cr+3.3Mo+16N), austenite/ferrite phase constitution, intermetallic phase precipitation and the cost based on property diagram via Thermocalc Tooling. The hot working temperature was optimised giving excellent surface quality qith crack free. The final products have been sucessfully produced in industry with excellent corrosion performance and the surface quality. Another example is regarding alloy design and continuous casting parameters for nickel saving austenitic stainless steels. Both the surface quality and the excellent cold formability are ensured through modification of chromium and manganese contents within the norminal chemical composion range based on Thermocalc Tooling.

Integration Framework and Usage - IIB

Wednesday PM
May 24, 2017

Room: Salon II, III
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

2:00 PM Invited

An ICME Framework for Incorporating Bulk Residual Stresses in Rotor Component Design: *Vasisht Venkatesh*[1]; [1]Pratt & Whitney

2:30 PM

Materials Integration System being Developed for Relating Among Process, Structure, Property, and Performance: *Masahiko Demura*[1]; Junya Inoue[1]; Makoto Watanabe[2]; Manabu Enoki[1]; Toshihiko Koseki[1]; [1]The University of Tokyo; [2]National Institute for Materials Science

Still now, process, structure, property, and performance are the key elements in materials science and engineering, and any types of modellings can be regarded as links relating among them. Building a chain of links among them and predicting performance should be helpful and would be crucial for accelerating the R&D of new innovative structural materials. Based on this guiding principle, we have proposed a new concept named Materials Integration (MI) and have been developing the MI system in the SIP* Structural Materials for Innovation program led by the Cabinet Office, Japan. It is a modular-type system, where one designs and executes a workflow connecting several computational modules of simulations, empirical or theoretical formulas, and experimental or computational databases. Each workflow can be regarded as a chain of modellings linking among the four elements, and yields an integrated pathway to predict the performance of a target structural part. In this talk, we will introduce our MI system with a couple of workflow examples for predicting creep lifetime of a heat-resistant engineering part. *SIP: Cross-ministerial Strategic Innovation Promotion Program.

2:50 PM

An Ontological Framework for Integrated Computational Materials Engineering: *Sreedhar Reddy*[1]; BP Gautham[1]; Prasenjit Das[1]; Raghavendra Yeddula[1]; Sushant Vale[1]; Chetan Malhotra[1]; [1]TCS Research, Tata Consultancy Services

ICME is expected to significantly reduce the dependence on trial and error based experimentation cycles for materials development and deployment in products. However, modelling and simulation is a knowledge intensive activity. In an integrated design, choosing right models for different phenomena, at right scales, with right parameters, and ensuring integration across these models is a non-trivial task. The gaps in modelling and simulation need to be filled with tacit knowledge and co-engineered with product knowledge. Therefore, an IT platform having capabilities such as, a) a repository of building-block models, templates and workflows with an intelligent means to choose and compose right workflows for a given problem, b) a knowledge engineering framework for knowledge management, c) a simulation services framework for simulation tool integration and simulation execution, d) tools for decision support, optimization, robust design etc., is essential for scaling up ICME for industrial applicability. This requires a unifying semantic foundation. Ontologies can provide the common substrate for integration of different models, the common language for information exchange, and the means for capturing and organizing knowledge. However, ontology engineering is a challenge when we consider the diversity of the material systems, products, processes and mechanisms involved in ICME. This calls for a flexible ontological framework that provides a means for modelling the generic structure of a subject area (e.g. materials) and a means for instantiating subject specific ontologies from this generic structure. We describe a model driven framework and how it has been used for developing an enabling platform for ICME.

3:10 PM

Establishment of a Vocabulary-inventory System for Data Utilization in Materials Science and Engineering: *Takuya Kadohira*[1]; Toshihiro Ashino[2]; Hiroaki Ishiki[3]; Satoshi Minamoto[1]; Kaita Ito[4]; Makoto Watanabe[1]; Junya Inoue[4]; Manabu Enoki[4]; Toshihiko Koseki[4]; [1]National Institute for Materials Science; [2]Toyo University; [3]ITOCHU Techno-Solutions Corporation; [4]University of Tokyo

We show an idea to construct systems of vocabulary-inventory for research and development of materials with data utilization. Based on the idea, the list of vocabularies with persistent identifiers will be created using collective intelligence, i.e. more than one user can register descriptors used in his/her research and organize them under his/her own data structure such as data schema, notes and so on. After evaluation of the idea using wiki, we have created an experimental system under the idea. In this talk, we will make a brief introduction about the experimental system, and also discuss a potential of the idea to establish an unified ontology for data integration from scattered data-sources, which will lead acceleration of data-utilized research in the field of Materials Science and Engineering.

3:30 PM Break

3:50 PM

Digital Infrastructure for Driving Rapid Insertion of New Materials: *Deborah Mies*[1]; Will Marsden[1]; [1]Granta Design, Ltd.

ICME was founded to drive the rapid insertion of new materials into parts manufacturing. The methodologies to achieve this have evolved dramatically in recent years with the evolution of additive manufacturing. New polymeric and metallic feed materials, for instance, are being developed at a rapid pace to meet the demands of this manufacturing method as well as new materials developed as a result of the manufacturing process itself. This digitally-driven manufacturing process can easily be integrated into a data management infrastructure that supports the capture and management of all process inputs and outputs, supports data discovery while securing IP, and enables certifiable knowledge extraction from integrated computational analysis tools. When execution is consistent with developing standards for certification, these new materials can be quickly approved for manufactured parts. Granta Design presents its experience in advancing the digitization of advanced materials development activities, such as ICME or Additive Manufacturing.

4:10 PM

Context Aware Information Retrieval from Materials Publications: Sapan Shah[1]; Dhwani Vora[1]; B P Gautham[1]; *Sreedhar Reddy*[1]; [1]TCS Research

Knowledge of material properties as a function of material composition and manufacturing process parameters is of significant interest to materials scientists and engineers. A large amount of information of this nature is available in publications especially in the form of experimental measurements, simulation outcomes, etc. In a typical problem solving context, when information required is not available in standard databases, an engineer has to first go through a large collection of publications, either internal reports or open literature, to filter the right set of documents, containing information relevant to the context. Having filtered the publications, an engineer has to then go through each of them to extract the relevant pieces of information. Our goal is to help automate some of these steps. In this paper, we present our ongoing work on a system that provides information search and extraction based on material entities such as elemental composition, manufacturing processes (along with processing parameters) and properties. To specify search criteria, the system provides a domain specific query language. The accuracy of our system critically depends on the accuracy of the information extraction component. To address this, we are developing a sophisticated extraction component that combines rule based and machine learning based approaches. We have conducted an experiment on a small library of publications on steel on which searches such as "get the list of publications about steel which has carbon composition between 0.2 and 0.3 and on which tempering is performed for about 30 to 40 min" are performed.

4:30 PM

Symbiotic Resources for Atomistic Simulations: nanoHUB + OpenKIM: *Sam Reeve*[1]; Christopher Chow[1]; Alejandro Strachan[1]; [1]Purdue University

Molecular dynamics (MD) simulations are increasingly being utilized within ICME frameworks and used by a wider range of the materials community. However, there are numerous potential issues in running MD simulations due to i) lack of computational resources or limited computational modeling and coding experience or ii) low level of access to interatomic models or difficulties in determining the ideal interatomic models. We describe the implementation and uses of an online simulation tool combining the capabilities of the nanoHUB and OpenKIM projects (both National Science Foundation supported). The Nanomaterials Mechanics Explorer (nanoHUB.org/resources/nanomatmech) leverages the cloud computing infrastructure and graphical user interfaces (GUI) of nanoHUB.org, alleviating the first set of difficulties. The tool internally queries the interatomic model database of openkim.org, shows the user all available potentials, downloads and builds the model chosen on the fly, and enables running MD simulations and directly comparing multiple models, addressing the second set of issues. The tool allows a wide range of user input (through the GUI), atomistic structure and thermodynamic outputs, and use the uncertainty quantification framework within nanoHUB, all within internet browsers, extending the usefulness further. In future work we hope to close the loop between nanoHUB and openKIM, using the nanomatmech simulations to provide properties (model predictions) and improve MD tests (standard calculation methods) available through OpenKIM.

4:50 PM

Ensuring Reliability, Reproducibility and Transferability in Atomistic Simulations: The Knowledgebase of Interatomic Models: *Ryan Elliott*[1]; Ellad Tadmor[1]; James Sethna[2]; [1]University of Minnesota; [2]Cornell University

Atomistic simulations using empirical interatomic potentials play a key role in realistic scientific and industrial applications. This talk describes an NSF-funded effort to develop an open source online tool for promoting the use and reliability of interatomic models. The Knowledgebase of Interatomic Models (https://openkim.org) allows users to compare model predictions with reference data, to generate new predictions by uploading simulation test codes, and to download models conforming to an application programming interface (API) standard that has been developed in collaboration with the atomistic simulation community. An overview will be given of the KIM project and its main components which include the KIM API, the KIM data structure for representing arbitrary material properties, the KIM processing pipeline, and the KIM visualization framework.

ICME Success Stories and Applications - II

Wednesday PM
May 24, 2017

Room: Salon IV
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

2:00 PM Invited
Making Materials Data Discoverable, Accessible, Interoperable and Reusable: Efforts at NIST: *Zachary Trautt*[1]; Sunil Bhaskarla[1]; Chandler Becker[1]; Mary Brady[1]; Carelyn Campbell[1]; Philippe Dessauw[1]; Alden Dima[1]; Lucas Hale[1]; Robert Hanisch[1]; Ursula Kattner[1]; Kenneth Kroenlein[1]; Chris Muzny[1]; Marcus Newrock[1]; Adele Peskin[1]; Raymond Plante[1]; Sheng-Yen Li[1]; Pierre-François Rigodiat[1]; Guillaume Sousa Amaral[1]; Xavier Schmitt[1]; James Warren[1]; Sharief Youssef[1]; [1]National Institute of Standards and Technology

There is increasing recognition of the need to improve the discovery, access, interoperability, and reusability of scholarly data, which is also a central aspect of the Materials Genome Initiative (MGI) [1]. Tremendous progress has been made in the five years since the launch of the MGI [2], specifically in the area of data discovery and access through the creation of materials resource registries and materials data repositories [3]. However, significant challenges remain in improving the interoperability and reusability of materials data. We will give a brief overview of NIST efforts in creating materials resource registries and materials data repositories, followed by a detailed overview of NIST efforts to: (i) facilitate the development of modular data schemas in materials science, and (ii) enable their discovery, access, interoperability, and reusability through the creation of a schema repository and registry. [1] Warren JA, Boisvert RF. Technical Report NIST IR 7898. [2] https://mgi.nist.gov/mgi-5th-anniversary-accomplishments[3] Dima A, Bhaskarla S, Becker C, Brady M, Campbell C, Dessauw P, Hanisch R, Kattner U, Kroenlein K, Newrock M, Peskin A, Plante R, Li S-Y, Rigodiat P-F, Amaral GS, Trautt Z, Schmitt X, Warren J, Youssef S. JOM 2016;68:2053.

2:30 PM
Computer-Aided Accelerated Development of Multi-phase TRIP-Assisted Steels: Shengyen Li[1]; Berham Basha[2]; Taymaz Jozaghi[3]; Miles Stopher[2]; Pejman Honarmandi[3]; Ibrahim Karaman[3]; Pedro Rivera Diaz del Castillo[2]; *Raymundo Arroyave*[3]; [1]National Institute of Standards and Technology; [2]University of Cambridge; [3]Texas A & M University

In this work, we present recent work on the accelerated development of a TRIP-Assisted Steel. The design framework builds (inverse) linkages connecting desired performance to microstructure (represented by phase constitution) and required chemistry and processing schedules. Specifically, recently develop thermodynamic and kinetic models connecting chemistry and heat treatment schedules (Intercritical Annealing, IA, and Bainite Isothermal Transformation, BIT) to phase constitution are coupled to models for the flow stress of composite microstructures based on irreversible thermodynamics of dislocation evolution are combined in order to establish chemistry/processing-microstructure-properties/performance relationships. These relationships are exploited within an evolutionary-based optimization framework to identify the optimal chemistry and processing conditions. The prescribed 'material recipe' is then verified experimentally. The kinetics of microstructure evolution during IA and BIT are characterized through conventional microstructural as well as dilatometry means. Phase constitution is evaluated and compared with computational predictions. Finally, the mechanical performance of the designed alloy/heat treatment protocol combination isevaluated.

2:50 PM
Multiscale, Coupled Chemo-mechanical Modeling of Bainitic Transformation during Press Hardening: *Ulrich Prahl*[1]; Mingxuan Lin[1]; Marc Weikamp[2]; Claas Hüter[3]; Diego Schicchi[4]; Martin Hunkel[4]; Robert Spatschek[2]; [1]RWTH Aachen University; [2]Research Center Jülich; [3]Max-Planck-Institute for Iron Research; [4]Stiftung Institut für Werkstofftechnik

Press hardening offers high strength components of light-weight vehicles. In conventional processes, the martensitic microstructure is obtained through in-tool quenching of austenite. With pre-heated tools, this process can produce bainitic microstructure with improved strength ductility balance. Modeling the phase transformation during this process is a challenging problem because of two reasons. First, there is a strong coupling between mechanical load, internal stresses, chemical composition and phase transformation kinetics. Due to the displacive nature of the bainitic transformation, a large eigenstrain is expected for the bainitic ferrite, which results in elastic/elastoplastic deformation in the microstructure. Second, Bainite is a hierarchical structure spanning three length scales. We model the coupled thermochemical and thermomechanical processes under various length scales. Large elastic deformations are described using ab initio and phase field crystal simulations and linked to macroscopic formulations of nonlinear elasticity. At the mesoscopic scale, the anisotropic migration of phase boundaries, the partitioning of carbon and the consequent carbide precipitation are modeled by a multi-phase field (MPF) method coupled with elastic and crystal plasticity models. The activation of different slip systems in both BCC bainitic ferrite and FCC austenite and the rotation of local orientation are emphasized in the crystal plasticity model. At the macroscopic scale, the transformation plasticity is modeled by a finite element method. The evolution of bainite is described by the Johnson-Mehl-Avrami equation parameterized by the phase field model from the lower length scale. Finally, tests on sheet specimens are used for validation of the numerical results.

3:10 PM
Development of Microstructure-based Multiscale Simulation Process for Hot Rolling of Duplex Stainless Steel: *Mototeru Oba*[1]; Sukeharu Nomoto[1]; Kazuki Mori[1]; Akinori Yamanaka[2]; [1]ITOCHU Techno-Solutions Corporation; [2]Tokyo University of Agriculture and Technology

Recent improvement of multi-phase field method enables us to simulate microstructure formed by various material processes and homogenization method attracts attention as the way of bridging microstructure and macro homogenized material properties. In this paper microstructure-based multiscale simulation by bridging various commercial software, not only multi-phase field method and homogenizaiton method but also nanoscale molecular dynamics simulation and finite element method, was applied to simulate hot rolling process of duplex stainless steel [S. Nomoto, et al., Integrating Mater. Manuf. Innovation, submitted]. Multi-phase field method software MICRESS coupled with CALPHAD (Thermo-Calc) database was used to simulate microstructure evolution by columnar and equiaxed solidifications during continuous casting. Elastic property for the constituent phases in the duplex stainless steel was calculated by molecular dynamics simulation and first principle calculation. Plastic property was obtained by nanoindentation tests. Homogenization calculation of HOMAT gives macro elastic property from microstructure and property of each phase and virtual material test performed by ABAQUS serves homogenized plastic property. With the material properties hot rolling process is simulated by dynamic explicit simulation of finite element method using ABAQUS. Recrystallization by hot rolling process was performed by multi-phase field simulation using MICRESS. The results are discussed to reveal the usefulness and problem for performing microstructure based multiscale analysis.

3:30 PM Break

3:50 PM

Implementing an ICME Approach to Design New Cu-Ni Alloys: *Eric Lass*[1]; Mark Stoudt[1]; Carelyn Campbell[1]; [1]National Institute of Standards and Technology

An Integrated Computational Materials Engineering (ICME) materials design approach was adopted to develop a "nickel-silver" alloy (Cu-Ni-Zn-Mn) with specific materials properties. Among the most important material properties were yield strength, work hardening behavior, electrical conductivity, color, and cost. In addition to the desired material properties, several processing constraints were considered, which included the effects of alloy composition and thermo-mechanical processing on the room temperature behavior. Experimental data collected from a series of test alloys were combined with available literature data to construct composition-dependent CALPHAD-type models of electrical conductivity and color. By employing the electrical conductivity model alone, a composition was identified in a single optimization cycle that met all alloy requirements except color. Incorporation of a color model resulted in the successful design of three alloy compositions possessing the requested combination of properties; and a series of additional, potentially more valuable alloys for future consideration.

4:10 PM

A Decision-Based Design Method to Explore the Solution Space for Microstructure after Cooling Stage to Realize the End Mechanical Properties of the Rolled Product: *Anand Blau Nellippallil*[1]; Vignesh Rangaraj[1]; Janet Allen[1]; Farrokh Mistree[1]; B.P. Gautham[2]; Amarendra Singh[3]; [1]The University of Oklahoma; [2]Tata Consultancy Services; [3]The Indian Institute of Technology, Kanpur

Manufacturing a product involves a host of unit operations and the end properties of the manufactured product depends on the processing steps carried out in each of these unit operations. In order to couple the material processing-structure-property-performance spaces, both systems-based materials design and multiscale modeling of unit operations are required followed by integration of these models at different length scales (vertical integration). This facilitates the flow of information from one unit operation to another thereby establishing the integration of manufacturing processes to realize the end product (horizontal integration).In this paper, we present a goal-oriented inverse, decision-based design method using the compromise Decision Support Problem construct to achieve the vertical and horizontal integration of models by identifying the design set points for hot rod rolling process chain. We illustrate the efficacy of the method by exploring the design space for the microstructure after cooling stage that satisfies the requirements identified for the end mechanical properties of a hot rolled product. Specific requirements like managing the banded microstructure to avoid distortion in forged gear blanks are considered for the problem. The method is goal-oriented as the design solutions after exploration of microstructure space are passed in an inverse manner to cooling and rolling stages to identify the design set points in order to realize the end product. The method is generic and has the potential to be used for exploring the design space of manufacturing stages that are connected to achieve the integrated decision-based design of the product and processes.

4:30 PM

A Computational Tool for Sand Casting of Welding Neck Flange: *Yinka Tanimowo*[1]; [1]University of Ilorin

Interactive user friendly software was developed in this study to facilitate the design and drafting of welding neck flange using sand casting process, thereby generating reliable data for use in manufacturing process. The software was developed using Microsoft Visual Studio (visual basic language).Accurate and efficient 3D (three dimensional) and 2D (two dimensional) detail working drawings of welding neck flange was generated by the software. The study considered the theoretical approaches in use for the design of welding neck flange using sand casting process and established a design analysis procedure for welding neck flange. The established procedure was implemented through the developed software such that a substantial saving in terms of time and cost of production of the design is obtained. The outcome of this research would enhance the designer's productivity by reducing the time required to analyze and document welding neck flange design results generated by the software shows very good agreement with that obtained through manual calculation using the established procedure. It was observed that the developed software successfully increase productivity over manual welding neck flange design and drafting by approximately eighty-three times in terms of the time required for the design.

4:50 PM

Crystal Plasticity Modeling and Experimental Validation of Deformation Response in Magnesium Alloy WE-43: Sriram Ganesan[1]; *Veera Sundararaghavan*[1]; [1]Department of Aerospace Engineering, University of Michigan-Ann Arbor

Magnesium alloys presents a wide array of unsolved scientific challenges such as the deformation response of the slip and twin systems, and the influence of dislocation interactions and twinning on tensile and fatigue behavior. A parallel 3-D crystal plasticity finite element (CPFE) open-source code has been developed based on a locally sensitive model of slip and twin system evolution. The single crystal response in this code is based on evolution laws for micro-scale state variables, namely, slip and twin system resistances. Scanning Electron Microscope (SEM)-Digital Image Correlation (DIC) experiments were conducted on WE-43 Magnesium alloys and the strain maps were compared to the corresponding maps obtained through the crystal plasticity finite element code by setting up a boundary value problem.EBSD maps of the measured microstructure were digitized to perform a quasi-2D plane stress simulation. Displacement boundary conditions were obtained from DIC results and the internal displacement distribution was predicted. The strain maps will serve to refine models for various hardening mechanisms in the Mg alloy (WE43) including interactions between crystallographic slip and twinning mechanisms. The multi-scale procedure for determining and validating polycrystalline response will also be highlighted in the presentation. The codes can be downloaded from https://github.com/prisms-center/plasticity

Verification, Validation, Uncertainty Quantification Issues and Gap Analysis

Thursday AM
May 25, 2017

Room: Salon I
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

8:00 AM

Uncertainty Quantification of Microstructural Variability Using an Analytical Approach: *Veera Sundararaghavan*[1]; Pinar Acar[1]; [1]University of Michigan

Pole figures and Electron backscatter diffraction (EBSD) scans are an important input for ICME models of thermomechanical processes. We derive an exact analytical formulation for uncertainty quantification (UQ) in material properties due to variability in microstructural measurements. The measurements are acquired from a set of Titanium alloy samples obtained by compressing a beta forged ingot followed by annealing. The samples were taken from different regions of the original ingot creating variability in the resulting microstructure. The joint multivariate probability distributions of the computed orientation distribution function (ODF) is found using the method of characteristic functions based on a Gaussian model of the pole figures. We also present an analytical solution to compute the uncertainty in linear elastic properties using the method of characteristic functions. Non-linear properties are treated analytically using direct transformation of random variables in the homogenization approach. Analytical methods provide a considerable reduction in computational times compared to numerical UQ methods. Thus, it is recommended that the presented approach be used as a first step to verify more advanced UQ models.

8:20 AM

Uncertainty Quantification in Microstructure Simulations of Thermal Conductivity and Fracture: *Michael Tonks*[1]; Marina Sessim[1]; Jie Lian[2]; [1]Pennsylvania State University; [2]Rensselaer Polytechnic Institute

A critical aspect of ICME is the development of tools that predict the impact

of microstructure on various physical parameters such as thermal conductivity and fracture. However, those tools are only useful if we can predict their uncertainty and validate their predictions. In this work, we use the DAKOTA code to predict the uncertainty of thermal conductivity and fracture models in the Multiphysics Object Oriented Simulation Environment (MOOSE). These uncertainties are then used to facilitate statistical validation of the models using microstructure data.

8:40 AM

Process Map-based ICME Approach to Fusion Welding in Titanium Alloys: *Yogesh Sovani*[1]; Chinnapat Panwisawas[1]; Magnus Anderson[1]; Richard Turner[1]; Jeffery Brooks[1]; Hector Basoalto[1]; [1]University of Birmingham

The Integrated computational materials science/engineering (ICME) initiative aims to establish the microstructure-property-processing relationships in challenging material design and component development. Variations of microstructure induced by liquid-solid interaction from laser fusion welding are responsible for the property scatter in the welded joints. In this paper, a process map-based ICME approach is developed to generate a design space for laser fusion welding of Ti-6Al-4V alloys. To rationalise the process variability, underlying physical effects at the mesoscale are simulated, and combined to provide a mesoscopic description for the process and hence feed into a mechanical simulation at the macroscale. Rapid melting, weld solidification microstructure, defect formation and micromechanics are modelled using representative temporal and spatial distributions to obtain the statistical information required to construct a property function for the macroscale simulation. A dislocation density based crystal plasticity model is then used to understand the flow behaviour of the weld microstructure using the representative volume elements (RVE) approach. It is demonstrated that scatter in material properties within the welded region has a significant impact on the weld structural integrity. The implications for the established process map, accounting for this property variation is discussed in relation to achieving a minimal-waste manufacturing route and the design criteria needed to obtain the functional integrity.

9:00 AM

Crystal Plasticity Parameter Estimation using Inverse Analysis: *Aritra Chakraborty*[1]; Philip Eisenlohr[1]; [1]Michigan State University

Crystal plasticity material models capture the anisotropic mechanical response of crystalline matter under load. Their underlying constitutive material descriptions have varying degree of rigorousness from purely phenomenological to dislocation mechanics-based. All such models include adjustable parameters that determine their efficacy in prediction. With increasing applications of structural materials in small scale applications where crystal plasticity material models play a vital role in predicting material deformation behavior, determination of their constitutive parameters becomes quintessential. A successful methodology of estimating model parameters has been through the inverse analysis which involves an optimization algorithm to minimize the error between simulated and experimental response. Moreover, these parameters are at the single crystal level, thus motivating such a comparison based on nanoindentation experiments that can capture the single crystal behavior efficiently. Even though this methodology has been of increased interest lately, a few questions remain unanswered: importance of the fitness function, stability and reproducibility of the methodology with crystal orientation, and the effect of the optimization algorithm selected. In this study, we aim to answer such questions. This work is supported by NSF grant DMR-1411102.

9:20 AM

Multi-scale Modeling of Anisotropic Behavior in Wrought Magnesium Alloys: *Baodong Shi*[1]; Chong Yang[1]; Yan Peng[1]; Jianliang Sun[1]; [1]National Engineering Research Center for Equipment and Technology of Cold Strip Rolling, Yanshan University

Texture induced strong anisotropy has impeded further application of wrought Mg alloys. This strong anisotropy cannot be fully captured by only macroscopic constitutive modeling with directional distortional hardening. Thus, a multi-scale modeling characterizing anisotropic mechanical behavior for Mg alloys was developed based on the concept of ICME in the current work. A bottom-top approach was employed to obtain material parameters from lower scale to neighboring larger scale to connect nano-, micro-, meso- and macro-scales. More precisely, molecular dynamics simulation in nano-scale was applied to obtain the coefficients for dislocation mobility in micro-scale; the hardening parameters of the crystal plasticity model in meso-scale were obtained by the dislocation dynamics simulation; stress-strain responses for wrought Mg alloy under non-proportional loading were computed by a CPFEM model in meso-scale, and further employed to verify a macro-scale internal state variable (ISV) model for characterization of anisotropic behavior. This multi-scale modeling was validated by comparison between evolution of yield surfaces and experimental observations under non-proportional loading for AZ31 Mg alloy sheet.

9:40 AM

Multiscale Modeling of Pure Nickel: *Shane Brauer*[1]; Imran Aslam[1]; Andrew Bowman[1]; Bradley Huddleston[1]; Justin Hughes[1]; Daniel Johnson[1]; William Lawrimore[2]; Luke Peterson[1]; Mark Horstemeyer[1]; [1]Mississippi State University; [2]Engineering Research and Development Center

A physically-based, multiscale modeling approach has been applied, in tandem with uncertainty quantification, to simulate three-point bending of pure nickel. Downscaling requirements are driven by the complex stress state induced by the three-point bend, which is experimentally obtained as a force-displacement. Those requirements are then met by upscaling from the atomistic length scale to the macroscale. Density functional theory was utilized at the electronic principal's scale to determine the lattice parameter and equilibrium energy of nickel (Ni), which were then upscaled to the atomistic scale. At the atomistic length scale the Modified Embedded Atom Method was used to calibrate the nickel energy potential curve, which was then used to simulate the motion of a dislocation and, subsequently, to determine the dislocation velocity. The dislocation velocity was then upscaled to the microscale to evaluate the hardening constants of nickel by utilizing Multiple Dislocation Dynamics Plasticity simulations. The hardening constants are upscaled as parameters used in Crystal Plasticity simulations to obtain the stress-strain curves for the three stress states, compression, tension, and shear. The stress-strain curves are upscaled to the macroscale and calibrated using the MSU-ISV Plasticity-Damage Model. The macroscale calibration is fed into Abaqus as a user material model in order to accurately replicate the three-point bending of a thin sheet of pure nickel. Uncertainty was quantified at each length scale as well as propagated throughout the length scales. The force-displacement data obtained from Abaqus is in good agreement with the experimental result.

10:00 AM Break

Phase Field Modeling - II

Thursday AM
May 25, 2017

Room: Salon II, III
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

8:00 AM

Three-dimensional Phase-field Crystal Simulation of Grain Boundary Migration, Grain Rotation and Grain Translation in Crystals: *Akinori Yamanaka*[1]; Kevin McReynolds[2]; Peter Voorhees[3]; [1]Tokyo University of Agriculture and Technology; [2]NIST; [3]Northwestern University

Grain boundary (GB) migration and grain rotation are important mechanisms for grain growth in nanocrystalline materials. In order to deeply understand these mechanisms, molecular dynamics (MD) simulations of grain coarsening and shrinkage driven by GB curvature have been often performed. Although MD simulations enable us to quantitatively investigate atomic motions in the vicinity of GBs, the timescale of MD simulations is too short to study the GB migration and the grain rotation in real timescales. On the other hand, the phase-field crystal (PFC) model has attracted much attention as a powerful methodology for simulating atomistic scale motion of GBs that occurs on diffusive timescales. In this presentation, we will report on three-dimensional (3D) PFC simulations of the shrinkage of a spherical grain embedded in a single crystal. The results clarify the structure and evolution of the dislocation network formed in the GB. We find that the evolution of the dislocation network strongly affects morphology and rotation of the embedded grain. Furthermore, the grain translation of a columnar grain in a tricrystal simulated by 3D PFC simulations will be presented.

8:20 AM

Parameterizing the Structural Phase Field Crystal Model Using Molecular Dynamics Data: *Jason Luce*[1]; David Montiel[1]; Katsuyo Thornton[1]; [1]University of Michigan

The structural phase field crystal (XPFC) model is used to study material phenomena at atomic length-scales and diffusive time-scales, bridging the gap between atomistic and mesoscale models. As a result of these properties, the XPFC model can be used to simulate the dynamic behavior of grain boundary structures. However, the XPFC model needs to be parameterized using experimental data or other computational results in order to simulate the properties of a specific material. One method by which the XPFC model can be parameterized is through changes to the two-body density correlation function (DCF), which is a term in the XPFC model's free energy functional. In the XPFC model, the DCF is approximated using one or more Gaussian functions. Previous work has shown that changing the height and width of the Gaussian function(s) in the XPFC correlation function can predictably alter the grain boundary energy (GBE) and structure in two-dimensional hexagonal systems. Building on these results, three-dimensional hexagonal close packed grain boundaries are created using the XPFC model, and the DCF is parameterized so that the GBEs agree with molecular dynamics simulations of magnesium grain boundaries (Mg) performed by Ni et al. [1]. This parameterized XPFC model will be used to study equilibrium and non-equilibrium phenomena associated with Mg grain boundaries. These results will be used as input for larger scale continuum models, e.g., phase field simulations, within an integrated computational materials engineering framework.[1] C. Ni, H. Ding, M. Asta, X. Jin, Scripta Materialia, 109 (2015), 94-99

8:40 AM

Parameter Estimation for Two Dimensional Phase-field Simulation using Ensemble Kalman Filter: *Kengo Sasaki*[1]; Akinori Yamanaka[1]; Shin-ichi Ito[2]; Hiromichi Nagao[2]; [1]Tokyo University of Agriculture and Technology; [2]Earthquake Research Institute, The University of Tokyo

In order to reproduce the microstructure evolution by a numerical simulation, the phase-field method is attracting much attention. While it has been applied for simulating various phenomena that occur in various materials, there are unknown parameters that strongly influence the simulation result. Moreover, phenomena such as phase transformation and grain growth etc. occur inside materials, consequently making it difficult to measure and determine such unknown parameters. Therefore, identification of suitable parameter is one of the critical issue for phase-field method to reproduce actual phenomena. Recently, we have developed a method to estimate such unknown parameters in the phase-field model from experimental measurements. In this study, the ensemble Kalman filter (EnKF), which is one of the sequential Bayesian filters commonly used in data assimilation, is applied to the phase-field simulation of austenite-to-ferrite transformation in Fe-C-Mn alloy. We have already validated its effectiveness in one dimensional simulation by performing the twin experiments, where synthetic experimental data created by the simulation model is used instead of the real measurements. Next, in order to apply for two dimensional simulation we have employed parallel computation using GPU since EnKF requires running a large number of simulation at the same time resulting in large computational cost. In this presentation, we are showing the result of parameter estimation for two dimensional phase-field simulation with different conditions.

9:00 AM

Strong Interfacial Energy Anisotropy in the PRISMS-PF Phase Field Model Code: *William Andrews*[1]; Stephen DeWitt[1]; Larry Aagesen[2]; Katsuyo Thornton[1]; [1]University of Michigan; [2]Idaho National Lab

Materials frequently exhibit interfacial energy anisotropy. When the anisotropy is sufficiently large, flat facets and sharp corners (edges) form in the equilibrium shape of a second-phase particle, and interfaces with unstable orientations undergo thermal faceting, the decomposition of thermodynamically unstable orientations into stable ones. Strong anisotropy poses two numerical challenges: flat facets and sharp corners are difficult to resolve, and thermal faceting is associated with mathematical ill-posedness. We have implemented and verified a phase field model with bulk diffusion and strong interfacial anisotropy that can generate nearly flat facets and that results in the expected corner (edge) and thermal-faceting behavior. The model retains well-posedness via the incorporation of a higher-order regularization term, which affects equilibrium shapes in a predictable way, and we omit the gradient penalty in concentration in order to reduce the order of the regularized equations. This model has been implemented in the phase field (PF) code developed within the Center for PRedictive Integrated Structural Materials Science (PRISMS), which is an open source phase field code that employs the deal.II finite element library. PRISMS-PF employs matrix-free elements, explicit time-stepping, and state of the art numerical and parallelization libraries to deliver high performance and scalability. The features and performance of the anisotropic PRISMS-PF applications will be discussed, including methods to easily implement anisotropy for different crystalline symmetries.

9:20 AM

Phase-field Approach for Predicting the Kinetics of Static Recrystallization in Ti-Al Alloys with Inputs from Experiments and Crystal Plasticity: *Arunabha Roy*[1]; Sriram Ganesan[1]; Anna Trump[1]; Susan Gentry[1]; Veera Sundararaghavan[1]; John Allison[1]; Katsuyo Thornton[1]; [1]University of Michigan at Ann Arbor

A three-dimensional (3D) computational framework has been developed to model recrystallization and grain growth phenomena in Ti-Al alloys by using the phase-field approach with inputs from a crystal plasticity model. In this framework, the evolution of the dislocation density during the deformation process of polycrystalline Ti and Ti-Al alloys is predicted using a 3D multiscale crystal plasticity finite element (CPFE) code. The grain structure from a phase-field simulation and experimental texture data from electron backscatter diffraction are used as the initial condition for a CPFE simulation. The CPFE simulation then provides the crystal orientation and dislocation density of each grain during the deformation of polycrystalline metals. The results are then used as the initial condition for a phase-field simulation of recrystallization. The kinetics of the microstructural evolution is analyzed by examining the recrystallized volume fraction as well as grain size distribution and grain morphology. The simulation results are compared with the experimental data for range of temperatures and alloy compositions to determine how those factors influence the microstructural evolution.

9:40 AM

Structure-property Relations in Annealing of Low carbon Steel: Trinath Gaduparthi[1]; *Gerald Tennyson*[1]; Ayush Suhane[1]; Srimannarayana P[1]; [1]TCS Research

Mechanical properties of interest such as yield strength, UTS, ductility etc.,are affected by the hierarchical features of the microstructure. This necessitates the use of multiscale approaches in a physics based simulation framework to obtain desired properties of the representative microstructure. However, a change in the process conditions results in a different microstructure of the material. This requires a rerun of the compute intensive multiscale simulations to obtain desired properties and may not be of utility when quick decisions have to be taken. Instead, a data-driven approach is more feasible to obtain properties corresponding to a changed morphology and composition of the microstructure. In the present work, representative microstructures and corresponding mechanical properties are generated for a low carbon steel (0.08 - 0.14 %C) during annealing for different processing conditions, initial composition and morphology. Phase field method is used to obtain the representative microstructures which are then used as input to micromechanics simulation to compute the properties. The obtained microstructures are digitally represented using two point statistics. To make the computations tractable the dimensions of the digitized microstructure are reduced using the principal component analysis (PCA) technique. Further to this, utilizing the PyMKS framework, polynomial regression is deployed on a sample set to obtain the structure-property relations which are cross validated using data derived from the sample set. The structure-property relations so obtained could be useful in the solution of the inverse problem of arriving at a process route for a desired material property.

10:00 AM Break

ICME Success Stories and Applications - III

Thursday AM
May 25, 2017

Room: Salon IV
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

8:00 AM

Integrated Experimental and Computational Studies of Non-conventional Transformation Pathways in Titanium Alloys: *Yufeng Zheng*[1]; Rongpei Shi[1]; Deep Choudhuri[2]; Talukder Alam[2]; Robert Williams[1]; Rajarshi Banerjee[2]; Yunzhi Wang[1]; Hamish Fraser[1]; [1]The Ohio State University; [2]University of North Texas

The precipitation of hcp alpha phase in bcc beta phase matrix is critical for titanium alloys due to its significant influence on mechanical properties. The nucleation of alpha phase can be affected strongly by the compositional and/or structural instabilities within the beta matrix and so may follow non-conventional transformation pathways. In this research, the pathways for refined and super-refined intragranular precipitation of the alpha phase in Ti-5Al-5Mo-5V-3Cr (Ti-5553) were studied coupling advanced modern characterization techniques and powerful computational simulation. Experimental results indicate clearly that during the as-quenched condition Ti-5553 being heated up rapidly to the ultimate aging temperature (600°C), refined alpha microstructure is produced in beta matrix by pseudo-spinodal decomposition mechanism in which large number of solute lean regions formed by thermal compositional fluctuation act as favorable sites of alpha precipitation. While on the other hand, during as-quenched condition Ti-5553 being heated up slowly, the pre-formed large number of nano-scale isothermal omega phase particles can assist subsequent super-refined alpha precipitation. Computational simulation using phase field modeling based on structural and compositional information obtained from experiment shows that the presence of such fine scale compositional and/or structural instabilities due to pre-formed solute lean region or the omega phase particles can modify the compositional and stress field in the parent beta matrix and therefore provide an additional driving force, and nucleation site, for alpha precipitation. A detailed understanding of non-conventional transformation pathways controlling refined and super-refined alpha microstructure in Ti-5553 will be described.

8:20 AM Invited

ICMSE for Titanium: A Status Report: *Dipankar Banerjee*[1]; John Allison[2]; [1]Indian Institute of Science; [2]University of Michigan

We examine in this presentation the current status of integrated computational materials science and engineering (ICMSE) of titanium alloys. We first explore the scientific core of computational materials science underlying various key phenomena that characterize the metallurgy of titanium alloys, within an integrated multiscale framework. Significant gaps in physics-based models continue to exist even as models evolve towards a greater computational and simulation capability. We then examine efforts directed towards the prediction of engineering properties that links key ingot to billet conversion process variables, microstructure and texture, and mechanical properties. These efforts are based on extraction of location-based data sets of strain, strain rate, and temperature that influence the evolution of structure and microtexture from billet to final forged samples. Engineering titanium alloys are largely based on relatively coarse two-phase bimodal stress. Stress and strain partitioning and crystal plasticity methodologies are used to model microstructure, texture and microtexture. Finally neural network methods predict property dependence using statistically characterized relationships. We note that computational materials science efforts for intermetallics of titanium alloys based on gamma aluminide are currently not extensive. Finally we describe current efforts directed at evolving towards next generation ICMSE tools that include integrated multiscale modeling frameworks, uncertainty quantification, rapid and quantitative experimental capabilities, information infrastructure and industry ready open source software for rapid insertion of new science.

8:40 AM

Through Process Modelling of Microstructure Development in AA6082 Extrusion Alloys: *Warren Poole*[1]; Mary Wells[2]; Nick Parson[3]; Jingqi Chen[1]; Yahya Mahmoodkhani[2]; [1]The University of British Columbia; [2]University of Waterloo; [3]Rio Tinto Aluminium

There is a complex interplay between the various processing steps in aluminum extrusion production which affect the properties of the final extrudates in service. For example, the role of microstructure development during homogenization has important effects on the grain structure of as-extruded products. This study is concerned with the variation of grain structure (including crystallographic texture) through the thickness of the extrudate and how this can affect the anisotropy of the mechanical response. It will be shown that by using finite element method models, the deformation path can be tracked as the material moves through the die and exits. This deformation path controls the formation of deformation and possible recrystallization textures which spatially vary through the thickness of the extrudate. In this work, extrusion trials have been conducted on AA3003 with a very high density of dispersoids to minimize recrystallization during extrusion and on conventional AA6082 to examine an industrially relevant alloy. The deformation texture at the centre and surface of the extrudate can be rationalized by the strain path the material follows as it passes through the die. In addition, it is found that details of the die geometry affect the surface layer and possible formation of a peripheral coarse grain (PCG) region. This has been rationalized by detailed EBSD, finite element method models and crystal plasticity calculations.

9:00 AM

ICME Approach to Microstructural Design of Corrosion-Resistant Aluminum Alloys: *Kenneth Smith*[1]; John Allison[2]; James Beals[1]; Rudolph Buchheit[3]; Gerald Frankel[3]; Lori Flansburg[4]; Jacquelynn Garofano[1]; Mark Jaworowski[1]; Jenifer Locke[3]; Amit Misra[2]; Anna Paulson[4]; Rajiv Ranjan[1]; Brian Said[4]; Christopher Taylor[5]; Katsuyo Thornton[2]; [1]United Technologies Research Center; [2]University of Michigan; [3]The Ohio State University; [4]Lockheed Martin; [5]DNV GL

Corrosion costs the U.S. over $1 trillion annually, yet is typically not analyzed at a detailed level during the product design phase. We are developing an ICME toolset to relate microstructure with corrosion performance for aluminum alloys that enables corrosion assessment in the design process. This effort combines modeling and experiment to ultimately provide risk assessment and service life predictions, combined with mechanical prediction models, to demonstrate microstructural design optimization. The current foci are a legacy aluminum alloy, AA-7075, and a newer Al-Li alloy, AA-2070. The approach links electrochemical and microstructural characterization of the surface to the microscale corrosion processes. The experimental electrochemical characterization includes optical microscopy, SEM, TEM, XRD, Scanning Kelvin Probe Force Microscopy, Microcell electrochemistry, and zero resistance ammeter measurements. The microstructure characterization techniques include a combination of optical microscopy, SEM, TEM, XRD, and EBSD. Additionally, high throughput screening for corrosion analysis is being developed that incorporates small scale experiments, and the analysis of exposed panels. These descriptions are unified through: a corrosion database; microstructure evolution models; a multi-physics microgalvanic corrosion model; a phase field model; and Bayesian models of pit growth. The validation and verification of the ICME tools uses corrosion pit formation on both salt fog cabinet exposed and outdoor exposed coupons. These tests will provide the input for future demonstrations on manufactured components, and demonstration of corrosion ICME toolset, to link corrosion exposure testing and modeling with design, life prediction, and certification requirements.

9:20 AM

A Thermo-mechanically Coupled Model to Predict Joint Properties in Friction Stir Scribe Welding of Dissimilar Materials: *Varun Gupta*[1]; Piyush Upadhyay[1]; Xin Sun[1]; Erin Barker[1]; Leonard Fifield[1]; Blair Carlson[2]; [1]Pacific Northwest National Laboratory; [2]General Motors

Joining process simulation is part of the ICME spectrum aiming at computationally linking the joining process parameters to the joint properties. The friction stir welding process is becoming increasingly common as a method to join dissimilar materials and has wide spread applications in several industries, including automotive, aerospace, robotics, shipbuilding and offshore energy production. The solid state nature of the process enables joining materials with significantly different physical properties. The present work focuses on the friction stir joining of fiber reinforced polymer composite to aluminum alloys. For welds in lap configuration, an enhancement to this technique, known as friction stir scribe (FSS), is made by introducing a short hard insert, referred to as cutting-scribe, at the bottom of the tool pin. The cutting-scribe induces deformation in the bottom plate material which leads to the formation of hook-like mechanical interlocks at the interface of the two materials. A thermo-mechanically coupled finite element model is developed to quantitatively capture the morphology of these interlocks formed during the FSS welding process. The identified interface morphology coupled with the predicted temperature field from this process-structure model can be used to estimate the post-weld microstructure and the associated joint strength. The computational model is used to study the effect of different process parameters including tool geometry, welding and rotational speed on the interfacial morphology and the resulting joint mechanical properties.

9:40 AM

First Principles (DFT) Calculation of Ti3B4 Elastic Constants: *Somnaang Rou*[1]; K.S. Ravi Chandran[1]; [1]University of Utah

Elasticity of strong borides, especially the independent elastic constants that are specific to the crystal structure, are important for the fundamental characterization of their mechanical behavior and physical properties. In this work, the nine-independent elastic constants of the new titanium boride compound, Ti3B4, having the orthorhombic crystal structure is determined rigorously using density functional theory based calculation approach. This was done through the strain energies as determined, for specific deformations, within WIEN2k utilizing full potential linear augmented plane wave (FLAPW) and generalized gradient approximation (GGA). It has been found that the polycrystalline Voigt-Reuss-Hill averages of the independent elastic constants, are quite high (E=492GPa, G=217GPa, B=224GPa, í=0.13) placing this boride very close to the well-known titanium diboride (E=570GPa, G=254GPa, B=249GPa, í=0.12). The elastic anisotropy of this compound, compared to TiB and TiB2 is comparable, exhibiting low levels of anisotropy. The calculated anisotropy about the {001} plane, however, exhibits notably increased levels of anisotropy due to the directionally dependent bonding of the hexagonal boride chains within the lattice. The same boride chains were found to be responsible for the high modulus, particularly in the [001] direction. Additionally, the charge densities were determined to cause electron accumulation near the boride chains, resulting in strengthening of the B-B chain bonds.

10:00 AM Break

Plenary IV

Thursday AM
May 25, 2017

Room: Salon II, III, IV
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

10:20 AM Invited

European Materials Modelling Council: *Nadja Adamovic*[1]; Pietro Asinari[2]; Gerhard Goldbeck[3]; Adham Hashibon[4]; Kersti Hermansson[5]; Denka Hristova-Bogaerds[6]; Rudolf Koopmans[7]; Tom Verbrugge[8]; Erich Wimmer[9]; [1]TU Wien; [2]Politecnico di Torino; [3]Goldbeck Consulting Limited; [4]Fraunhofer Institute for Mechanics of Materials IWM ; [5]Uppsala University; [6]Dutch Polymer Institute; [7]Koopmans Consulting; [8]DOW Benelux B.V.; [9]Materials Design SARL

The aim of the EMMC is to establish current and forward looking complementary activities necessary to bring the field of materials modelling closer to the demands of manufacturers (both small and large enterprises) in Europe. The ultimate goal is that materials modelling and simulation will become an integral part of product life cycle management in industry, thereby making a strong contribution to enhance innovation and competitiveness on a global level. Based on intensive efforts in the past two years within the European Materials Modelling Council (EMMC) which included numerous consultation and networking actions with representatives of all stakeholders including Modellers, Software Owners, Translators and Manufacturers in Europe, the EMMC identified and proposed a set of underpinning and enabling actions to increase the industrial exploitation of materials modelling in Europe. EMMC will pursue the following overarching objectives in order to establish and strengthen the underpinning foundations of materials modelling and bridge the gap between academic innovation and industrial application: 1. Enhance the interaction and collaboration between all stakeholders engaged in different types of materials modelling, 2. Facilitate integrated materials modelling in Europe building on strong and coherent foundations, 3. Coordinate and support actors and mechanisms that enable rapid transfer of materials modelling from academic innovation to the potential beneficiaries in industry, 4. Achieve greater awareness and uptake of materials modelling in industry, in particular SMEs,5. Elaborate Roadmaps that (i) identify major obstacles to widening the use of materials modelling in European industry and (ii) elaborate strategies to overcome them.

11:00 AM Invited

Workforce Development for Materials Science & Engineering of the Future: *Katsuyo Thornton*[1]; Mark Asta[2]; [1]University of Michigan; [2]University of California, Berkeley

Modeling and simulation have become a key component of materials science and engineering, and computational tools are becoming more accessible and abundant. To take full advantage of these resources, workforce development in the field of computational materials science and engineering must be extended to those who do not specialize in computational approaches. This talk will begin with review the state of computational materials education and training, summarizing the various programs around the United States. A few of the programs will be highlighted, including the NSF-sponsored Summer School for Integrated Computational Education that facilitates the implementation of computational modules within existing required MSE curriculum. The talk will conclude with a discussion on potential approaches to reach a broader community, including those already in the workforce.

11:40 AM Concluding Comments

Poster Session

Monday PM
May 22, 2017

Room: Salon V, VI
Location: Ann Arbor Marriott Ypsilanti at Eagle Crest

P-3: A Diffusion Database for Multicomponent Cu Alloy: *Yong Du*[1]; Yuling Liu[1]; Shuhong Liu[1]; Dandan Liu[2]; Peng Deng[1]; Huixin Liu[1]; Qianhui Min[1]; [1]Central South University; [2]Central South University and Chinese Academy of Sciences

Owing to the excellent conductivity and outstanding plasticity, Cu alloy is widely used as a basis material. An accurate diffusion database is the key to realize the description of microstructure evolution of Cu alloy. The atomic mobility database for fcc phase in multicomponent Cu alloy was established via the DICTRA (DIffusion Controlled TRAnsformation) software package. The mobility parameters of fcc phase were constructed based on our new experimental diffusivity data, literature data and semi-empirical method. A case study for diffusivity in fcc Cu-Ni-Si alloys is demonstrated. By means of the solid-solid diffusion couples together with the electron probe microanalysis technique and Matano-Kirkaldy method, the composition dependence of ternary interdiffusion coefficients in Cu-rich fcc Cu-Ni-Sn alloy at 1073, 1023 and 973 K were measured. Based on the experimentally determined mole fraction interdiffusion coefficients as well as thermodynamic description of fcc phase, atomic mobilities of fcc phase in the Cu-Ni-Sn system were assessed by means of DICTRA. The newly obtained parameters were incorporated in the established database. The quality of the database was verified by comprehensive comparisons between various model-predicted diffusion properties and the experimental data. The general agreement validates the potential application of the present atomic mobility database to simulate the diffusion phenomenon in higher order systems.

P-8: Applications of Atomistic Simulations to Predict Phase Separation Diagram of Thermoplastic-toughened Epoxy Resins: Chunyu Li[1]; *Alejandro Strachan*[1]; [1]Purdue University

Thermoset polymers are widely used in aerospace and automotive industries as the main structural matrix for fiber composites because of their advantages in thermomechnical properties and easy and quick curing process. However their toughness, which is an important measure of material resistance to failure, is normally not satisfactory. Thus various methods have been utilized to modify epoxy resins in order to improve their toughness. One of the most common methods is the incorporation of a second phase, either rubbers or thermoplastics, into an epoxy resin. The final toughness of the toughed epoxy matrix depends on the phase morphology which is the result of reaction-induced phase separation in the curing process.A fundamental understanding of the reaction-induced phase separation is of great interests to the material community as well as industries. Molecular modeling is a powerful technique for getting such a understanding. Although there have been numerous efforts in studying phase separation of polymer blends by molecular modeling, few has been done on reaction-induced phase separations. In this presentation, we will report our recent efforts in predicting phase separation diagram by atomistic simulations for an epoxy system enhanced by thermoplastics. The procedure involves calculations of the solubility parameters, cohesive energy density and free energy of mixing for different compositions under different temperatures. Therefor, tremendous computer resources are required. The details, including algorithms and validations, will be presented in this talk. Our calculations indicate the phase separation diagram is predictable by atomistic simulations for reaction-induced phase separation.

P-10: Automating Thermodynamic Database Development with ESPEI: *Brandon Bocklund*[1]; Richard Otis[1]; Zi-Kui Liu[1]; [1]Pennsylvania State University

There are currently several public repositories of materials data that are actively developed, but no solution exists to utilize this data for automated CALPHAD modeling at scale. ESPEI is an open-source software package being developed to automate the construction of thermodynamic databases from first-principles and thermochemical data. ESPEI is built upon the open-source Python package pycalphad, which solves the multi-component, multi-phase Gibbs energy minimization problem. The main advantages ESPEI has over traditional modeling techniques are the automated selection of a model for the system being assessed and the propagation of quantified uncertainty through the calculations. This presentation will show the progress in the development of ESPEI by demonstrating its use in the assessment of a real system. The challenges and future potential of ESPEI will be addressed.

P-11: Bayesian Optimization of Superalloy Designs: *Joseph Licavoli*[1]; Paul Sanders[1]; Santu Rana[2]; Sunil Gupta[2]; Vu Nguyen[2]; Svetha Venkatesh[2]; [1]Michigan Technological University; [2]Deakin University

Experiments, real or via computationally intense simulation, are expensive both in terms of time and cost. Bayesian optimization is a machine learning approach to efficiently find the extremum in expensive systems with a small number of experiments. An unknown function underlying the system is first approximated using a Gaussian process. This gives a probabilistic mechanism to record data from finished experiments and fill in unexplored regions. Second, a pay-off function encodes a risk-taking strategy to evaluate each unexplored region based on their potential to return a better experimental outcome. Finally, the location of the pay-off function maximum is sought and recommended for the next virtual experiment. The Gaussian process is then refined, a new pay-off function is computed and the setting for another virtual experiment is obtained. This is continued until an acceptable outcome is reached. Bayesian optimization was combined with the CALPHAD method to search for new eta strengthened and high entropy nickel superalloys. Various criteria including volume fractions of strengthening phases (either eta or gamma prime), volume fractions of detrimental phases, and the solvus of strengthening phases were balanced in a weighted objective function. Optimized alloys were produced using vacuum induction melting (VIM) and were fabricated into slabs for preliminary evaluations. X-ray diffraction was used to verify CALPHAD predictions. The alloys were then evaluated for their mechanical properties and the properties relative to commercial alloys are discussed.

P-12: Bioinspired Computational Design of Novel Materials and Structures: *Iwona Jasiuk*[1]; Christopher Kozuch[1]; Srikanth Raviprasad[1]; [1]University of Illinois at Urbana-Champaign

Biological materials have excellent properties for their designated functions. General characteristics of biological materials are that they self-assemble and self-organize from atomic level into complex hierarchical, composite, often porous, and fluid filled structures. They are multifunctional, they adapt to environment and can often self-heal. We study various biological materials, ranging from hard mineralized tissues such as bone, nacre, enamel or turtle shell, to soft tissue such as cartilage, tendons, skin and others, to learn from nature and design new materials for various technological applications. We first present several cases illustrating how nature has optimized materials structures to yield superior and robust properties. One example is bone which has excellent structural characteristics: it is stiff, strong, tough and light. These highly desired properties for many structural applications are due to a composite and hierarchical structure of bone. Bone is a nanocomposite consisting of polymers and ceramics and pores. We conduct this study computationally, by using various tools from mathematics, physics, chemistry and engineering, such as topology optimization, micromechanics methods, and percolation. We explore concepts of hierarchy, fractality and other bioinspired structural designs to design new materials with superior mechanical, electrical and thermal performances, filling upper left corner in various Ashby property diagrams. The studied materials include lightweight yet stiff and strong materials, impact resistant materials, and electrically conductive polymers.

P-13: Bridging the Gap between Bulk Properties and Confined Behavior using Finite Element Analysis: *David Linder*[1]; John Ågren[1]; Annika Borgenstam[1]; [1]KTH - Royal Institute of Technology

Theoretically and empirically based models of materials properties are crucial tools in development of new materials; however, these models are often restricted to certain systems due to assumptions or fitting parameters. When expanding a model into alternative systems it is therefore necessary to have sufficient experimental data. When working with composite or highly confined materials, such as layered structures or coatings, this can be problematic as most available data is on bulk materials. The present work displays the potential of using Finite Element Method (FEM) simulations as a tool to understand

experimental observations and expand existing models to new systems using only bulk properties of the constituent phases. The present work focuses on the effect of geometrical constraints on the indentation behavior of elasto-plastic materials as an example on how FEM may be used to better understand experimental observations in composite or layered materials. The results may also be integrated into phenomenological models, expanding their application range.

P-14: Coexistence of Security, Flexibility and Productivity for the Materials Integration System: *Kaita Ito*[1]; Satoshi Minamoto[2]; Takuya Kadohira[2]; Makoto Watanabe[2]; Masahiko Demura[1]; [1]The University of Tokyo; [2]National Institute for Materials Science

Acceptance of software and experimental data from wide variety of sources is important for sustainable growth of the Materials Integration (MI) system. At this point, information security i.e. information leak prevention is essential for protection of intellectual property of the developer of software and the owner of data. However, guarantee of sufficiently high level of information security is difficult for researchers of materials science and engineering who are developing software but not not always an expert on information technologies. Therefore, security assurance must be equipped in the back-end of the MI system. Meanwhile, flexible accessibility and connectivity are also important for quick development of software and workflow in the MI system. To this end, MI-API (application program interface) is developing for unification of the I/O procedure of software and data. However, at least until the MI system become popular, the most of conventional software is not developed with MI-API. Therefore, unique I/O specification of software is wrapped so that it may be compatible with MI-API and to work as a module in the MI system. This wrapped software keeps the maintainability for original author of the software because the internal software itself is not touched. In this report, the concept, implementation and some specific examples of the workflow subsystem in the MI system is introduced. The MI system with modularized software and unified API enables the coexistence of security, flexibility and productivity for development of new materials.

P-18: CSUDDCC2: An Updated Diffusion Database for Cemented Carbides: *Yong Du*[1]; [1]Central South University

Cemented carbides are widely used in industry as cutting tools, wear parts, as result of the high hardness and good toughness. A reliable diffusion database is critical to simulate microstructure evolution of gradient cemented carbides and cellular cemented carbides, which have better performance and longer service lifetime than traditional cemented carbides. In 2014, we established version one of CSUDDCC1: a diffusion database for multicomponent cemented carbides [Weibin Zhang, Yong Du, et al., Int. J. Refract Met Hard Mater., 43,164-180 (2014)]. In this work, a description for the updated diffusion database CSUDDCC2 is presented. The atomic mobility database for fcc and liquid in C-W-Co-Fe-Ni-Cr-V-Ti-Ta-Nb-Zr-Mo-Al-N cemented carbides was established based on our new experimental data, literature data, first-principles calculation and theoretical assessment via the DICTRA (Diffusion Controlled TRAnsformation) software package. The atomic mobility parameters in liquid are theoretically calculated by the newly modified Sutherland equation, and the atomic mobility parameters in fcc phase are optimized by the diffusivities measured in the present work and from the literature. The mobility parameters for self-diffusion and impurity diffusion in metastable fcc structure were determined through a semi-empirical method or first-principles calculations. Comprehensive comparisons between calculated and measured diffusivities indicate that most of the experimental data can be well reproduced by the currently obtained atomic mobilities. Combining the thermodynamic database for cemented carbides, the diffusion database has been used to simulate the microstructure evolution during sintering of gradient cemented carbides and cellular cemented carbides. The simulated microstructure agrees reasonably with the experimentally observed one.

P-21: Development of Nb-Bearing Cast Austenitic Steels for Exhaust Components of Gasoline Engines: Hailong Zhao[1]; Yinhui Zhang[2]; Carlos Engler-Pinto[3]; Larry Godlewski[3]; Jacob Zindel[3]; Mei Li[3]; *Qiang Feng*[2]; [1]University of Science and Technology Beijing / Ford Motor Company; [2]University of Science and Technology Beijing; [3]Ford Motor Company

To comply with the stricter fuel consumption regulations, exhaust components for automotive gasoline engines are required to withstand exhaust gas temperatures as high as 1050\176C. Thus, it is urgent to develop advanced cast steels with higher heat-resistance. Our previous studies indicated the properties of these alloys could be strengthened efficiently by minor additions of C and N, which were also expected to improve their economic competitiveness. Then a series of Nb-bearing cast austenitic steels with variations of N/C ratio were designed through the complementary CALPHAD and experimental approaches. Three microstructural models were established based on the morphology of primary Nb(C,N), which changed from “Chinese-script” to mixed flake-blocky and faceted-blocky with increasing the N/C ratio. The creep, fatigue and oxidation behavior of three types of model alloys were investigated in the temperature range of 600\176C and 1000\176C. All best properties occurred in alloys with “Chinese-script” Nb(C,N), which could effectively strengthen grain boundaries and interdendritic regions. The precipitation and coarsening of Cr-rich phases (residual \948-ferrite and $(Cr,Fe)_{23}C_6$) were found to degrade creep and fatigue properties. Moreover, the fatigue mechanism was sensitive to testing temperatures, associated with the formation of subgrains at elevated temperatures, while the creep mechanism was sensitive to some microstructural features. Oxidation resistance was dependent on the as-cast microstructure and Si content. It is suggested that the development of cast austenitic steels could be achieved through the formation of “Chinese-script” Nb(C,N) and the elimination of Cr-rich phases as well as the prevention of carbide degeneration, based on ICME alloy design.

P-22: Experimental and Numerical Study of Secondary Dendrite Arm Spacing in a New Aluminum Alloy: Huimin Wang[1]; *Emre Cinkilic*[1]; Alan Luo[1]; Xinyan Yan[1]; [1]The Ohio State University

EZCastTM, a new cast aluminum alloy developed by Alcoa, offers excellent castability, thermal stability, low shrinkage and superior mechanical properties for structural applications. Secondary dendrite arm spacing (SDAS) formed during casting processing has a significant impact on the mechanical properties of this new alloy. Accurate prediction of SDAS is an important link in the Integrated Computational Materials Engineering (ICME)-based casting design using location-specific mechanical properties. In this study, casting experiments using a step die were carried out to establish a relationship between SDAS and cooling rate for EZCastTM. A numerical model was developed based on Kattamis-Flemings’s theory and the experimental results in this study, and successfully incorporated into a commercial casting simulation package.

P-23: Facilitating ICME through Platformization: B Gautham[1]; Sreedhar Reddy[1]; Prasenjit Das[1]; *Chetan Malhotra*[1]; [1]TRDDC, TCS Research, Tata Consultancy Services

Integrated Computational Materials Engineering (ICME) is poised to change the way we conduct engineering design in the future where product engineering will be carried out in close association with materials and manufacturing engineering. This is already being manifested in newer technologies such as additive manufacturing and composite materials where the boundaries between product and process and material are sufficiently blurred. In order to successfully leverage ICME, we need a platform that should allow for the seamless integration of product design with process design and materials design and should allow for all three to be investigated, analyzed and optimized simultaneously to be able to obtain the right material for the right product to be manufactured in the right way. It should also provide for a unified and flexible language for expressing the problem domain and allow for the integration of modeling and simulation tools, product and materials databases as well as machine learning, data analysis and optimization algorithms into the design process. Most importantly, such a platform should be context aware and knowledge enabled. It should provide a strong semantic basis for expressing and capturing knowledge related to the problem domain and a means to reason with this knowledge in a context-sensitive manner to provide context appropriate guidance to the designer during the design process. The current paper proposes a basic structure for such a platform and how it is being realized as TCS-PREMAP.

P-25: First Principles Study of Grain Boundary Segregation and Embrittlement of Sp-elements on bcc Fe: *Kazuma Ito*[1]; Hideaki Sawada[1]; [1]Nippon Steel & Sumitomo Metal Corporation

P,S,Sn and Sb have been well known as elements that segregate at grain boundaries and embrittle grain boundaries in Iron. However, the mechanisms have not been well clarified so far. In particular, although the mechanisms of segregation and embrittlement were discussed based on atomic-size effect or chemical effect, it has not been clear that how much these factors affect the segregation and embrittlement, respectively. In this study, we calculated the segregation energies and embrittling energies of P,S,Sn and Sb at sigma 3(111)/[110] tilt Fe grain boundary and evaluated the atomic size effects and chemical effects on these energies quantitatively by means of first-principles calculation. The results of segregation energies showed that chemical effects strongly enhance the segregation of P,S,Sn and Sb and atomic size effects cause the difference of the most stable segregation site between P,S and Sn,Sb. It is indicated by our calculation of embrittling energies that chemical effect on embrittlling energy increases for the elements with more p electrons, for example, from Sn to Sb or from P to S and atomic size effect on the energy increases for the elements with larger principal quantum number, for example, from P to Sb.

P-27: High Throughput Determination of Melting Temperatures of Molecular Systems: *Ka-Ming Tam*[1]; Nicholas Walker[1]; Brian Novak[1]; Dorel Moldovan[1]; Mark Jarrell[1]; [1]Louisiana State University

Determining the melting temperature remains an important challenge in the simulation of molecular systems. The conventional method based on stabilizing the coexistence of liquid and solid requires rather large system sizes. The continuous growth of computing power has come to a point where the coexistence method can be routinely done for systems described by classical force fields. However, this remains problematic for ab-initio simulations as they are often restricted to small systems of a couple hundreds of atoms. Given this limitation, it is clear that methods which can extract the thermodynamic melting point from small finite size systems is crucial especially when a reliable classical force field is not readily available. The first order transition, in which melting is a prominent example, has been studied in the context of statistical physics models. We employ some of these techniques to predict the melting point. A key concept of understanding the phase transition is in the energy distribution. We studied the energy distribution of molecular systems by calculating the ratios of different order cumulants. They show behaviors as expected for the first order transition and thus finite size scaling can be used to extract the transition temperature. In contrast to the conventional coexistence method, large system sizes are not necessary. The prediction can be systematically improved by better sampling of the energy distribution, which allows efficient high throughput parallel calculations and thus suitable for use in workflows used to optimize materials properties.

P-28: Image-based 3D Modeling of Aggregated Grains in Aluminium Alloy from High-resolution Synchrotron Radiation CT: *Masakazu Kobayashi*[1]; Yoshitaka Yabumi[1]; Hiroyuki Toda[2]; Osamu Kuwazru[3]; Hiromi Miura[1]; [1]Toyohashi University of Technology; [2]Kyushu University; [3]Fukui University

To understand inhomogeneous deformation of grain microstructure is one of important issue for metallic material design, because the development of inhomogeneity concerns the origins of yielding, fracture and recrystallization. In this study, 3D plastic strains during tensile deformation and grains shapes have been investigated in aluminium alloy by using synchrotron radiation CT. Furthermore, image-based grain microstructure models for crystal-plasticity finite element analysis have been developed to understand effects of neighbor crystallographic orientation and grain shapes on inhomogeneous deformation.

P-29: Integrated Computational Materials Engineering Development and Application in Materials Qualification: *Guofeng Chen*[1]; [1]CT, Siemens Ltd., China

The Materials Qualification (MQ) is defined as "The process of establishing that a given material is of sufficient quality. This generally involves testing, analysis, and establishment or confirmation of standards or requirements". In this paper, the applications of MQ are specifically exemplified for the materials development and application through Integrated Computational Materials Engineering (ICME) process, and some methodologies have been described to further improve the understanding of MQ technology execution and application in the new discipline of materials science and engineering.

P-30: Integrating microstructure-based properties into structural optimization of cast metal and injection moulded polymeric components: *Jakob Olofsson*[1]; Kent Salomonsson[1]; Joel Johansson[1]; [1]Jönköping University, School of Engineering

In outdoor power products as well as in the automotive area, the request for lightweight structures increases constantly. To identify high performing load bearing structures with low weight, low density materials (as glass fibre reinforced polymers (GFRP), aluminium and magnesium) as well as with high strength and density, as cast irons, needs to be considered. While all these materials have their separate microstructural characteristics to consider on multiple-scale levels, the industrial virtual product development process needs to be able to treat all these alternatives and production routes using a common simulation strategy, and integrate multiple aspects of design, structural analyses, manufacturing and multi-scale models into an integrated computational optimization approach.The current work aims to introduce a newly developed geometry optimization procedure that has been developed and implemented for GFRP as well as cast materials. An essential part of the approach is the modelling of microstructural features found on sub-scale levels and their effect on the local material behaviour and performance. By applying knowledge-based engineering in an ICME approach, an integrated and automated multi-objective optimization scheme has been established and implemented. For GFRP, the injection moulding process and its effect on glass-fibre orientation and material performance is modelled. For cast materials, casting process simulation including solidification, microstructure modelling and heterogeneous material characterization is applied. In the present contribution, the approach is outlined and discussed.

P-31: JARVIS: High-throughput Classical and Quantum Calculation Database for Materials: *Kamal Choudhary*[1]; Francesca Tavazza[1]; [1]National Institute of Standards and Technology

JARVIS is classical and quantum calculation for material properties. The goal of the classical part (JARVIS-FF) is to evaluate and compare the materials properties using interatomic potential through an easy to use web-interface. At present JARVIS-FF consists of more than 3800 Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) calculations (>16000 sub-calculations) using existing interatomic potentials for elastic, energetics, surface, vacancy formation energies and phonon properties of materials. The goal of the quantum part is to make density functional theory (DFT) calculation database for 2D-materials, thermoelectrics and solar-cell materials. The calculated properties of interest are structural, vibronic, electronic band-structure, optical, thermoelectric and elastic properties. At present JARVIS-DFT consists of more than 873 Vienna Ab-Initio Simulation Package (VASP) calculations (>25000 sub-calculations). Both JARVIS-FF and JARVIS-DFT are still evolving. All the input files used in the JARVIS-FF and JARVIS-DFT are available for public use to enhance data reproducibility. Statistical learning is used to find trends in the data. The JARVIS-FF is available at http://www.ctcms.nist.gov/~knc6/periodic.html and the JARVIS-DFT is available at http://www.ctcms.nist.gov/~knc6/JVASP.html . JARVIS is a part of Materials Genome Initiative (MGI) at NIST.

P-32: Local Structure Analysis via Voronoi Topology: *Emanuel Lazar*[1]; Jian Han[1]; David Srolovitz[1]; [1]University of Pennsylvania

A major challenge in atomistic simulation studies of defects in crystalline materials is their automated identification and characterization. Simulations today may contain billions of atoms, and identifying even simple vacancies can be difficult in highly perturbed systems, requiring artificial modification of data through quenching. We introduce an efficient and versatile technique, based on Voronoi cell topology, that enables auto- mated visualization, characterization, and analysis of complex defect structure, even at temperatures near melting.

P-33: Materials Integration System for Prediction of the Performance for Inhomogeneous Structural Materials: *Satoshi Minamoto*[1]; Takuya Kadohira[1]; Kaita Ito[2]; Makoto Watanabe[1]; Masahiko Demura[2]; [1]National Institute for Materials Science; [2]The University of Tokyo

A project of the Structural Materials for Innovation (SM4I) as a subject of the Strategic of Innovation Program (SIP) has started since 2014 as 5 years project. Here we aim to reduce time of development of new materials by developing

an integrated system for materials science (Materials Integration (MI) system). To this end, not only combination of various software for materials science, but also applying machine learning technique, data science and experimental data stored for many decades are crucial to treat various problems. Normally structural materials are inhomogeneous, then uncertainty is not negligible to understand the performance of the materials, while the uncertainty makes difficult to find appropriate pathways of the calculations and get robust answer. Then an integrated environment for materials science connecting many kinds of analysis technique is required to accelerate the speed of materials development by understanding the performance of the materials, such as fatigue life limit, crack propagation, toughness and so on. Furthermore finding and describing a relation among vocabularies enable us to connect prediction models more flexibly with less effort. In the presentation, features of the MI system will be shown and we discuss a possibility of the MI system.

P-34: Mechanical Properties of Novel Architectured Foams: *Diab Abueidda*[1]; Rashid Abu Al-Rub[2]; Iwona Jasiuk[1]; [1]University of Illinois at Urbana Champaign; [2]Masdar Institute of Science and Technology

Exploring new lightweight yet strong materials is of great scientific and industrial interest. Therefore, researchers have used different methods to develop such materials with the purpose of filling the upper left corner region of Ashby strength/density and stiffness/density charts. One should take into consideration how the cellular materials are interconnected. Structures possessing joints between their elements will have stress concentration which may lead to earlier collapse of the structures. In this paper, we created 3D cellular materials that are based on mathematical surfaces called triply periodic minimal surfaces (TPMS). Their structures do not possess any joints in order to minimize the effect of stress concentration. Additive manufacturing is used to construct the cellular materials, with a density below 50 kg/m3. We study their mechanical behavior through a series of computations and experiments. Finite element method is used to investigate the mechanical response of such cellular materials. Two finite deformation elastic/hyperelastic-viscoplastic constitutive models that are calibrated based on the mechanical response of the base material are used in the computational study of the TPMS-foams for validation and further analysis. They are Arruda-Boyce (AB) model and parallel network (PN) model. The AB model includes an initial linear elastic behavior whilst the adopted PN model includes an initial hyperelastic behavior. Both models include yielding and viscoplastic deformation. Then, these models are used in the finite element analysis to computationally study of the mechanical behavior of the cellular materials. Various TPMS architectures and densities are considered.

P-35: Microstructurally Short Fatigue Crack: Modeling Grain Boundary Effect and Crack Growth Rates: *Shardul Panwar*[1]; Veera Sundararaghavan[1]; [1]University of Michigan

Microstructurally short fatigue cracks play an important role in determining fatigue life of metal alloys. Thus, understanding the underline mechanism behind these cracks is important for accurate prediction of the fatigue behavior of these materials. We have developed a semi-analytical method, which is based on Bilby, Cottrell, and Swinden dislocation theory, to predict microstructurally short fatigue crack growth. In this theory, the plastic zone in front of the crack tip is represented as a continuous distribution of dislocations. In our approach, we assume that the stress produced by these dislocations is a function of the crack sliding displacement. When a microstructurally short crack reaches a grain boundary, it can either be blocked or retarded. To model this behavior, we have used a recently developed phenomenological grain boundary model. We show examples that compare our model's predictions with experimental results.

P-36: Microstructure Engineering of the Weld Heat Affected Zone in Line Pipe Steels: Thomas Garcin[1]; *Matthias Militzer*[1]; Warren Poole[1]; [1]The University of British Columbia

State-of-the-art line pipe steels are microalloyed low-carbon steels that combine high strength and fracture toughness with good weldability. During welding the heat affected zone (HAZ) experiences rapid thermal cycles resulting in a graded microstructure that can be significantly different from that of the base metal. Based on systematic experimental studies a microstructure evolution model has been developed for selected line pipe grades to describe austenite grain growth, dissolution of Nb(C,N) precipitates and the austenite decomposition kinetics into complex mixtures of irregular ferrite, upper and lower bainite and martensite/austenite (M/A) constituents for HAZ thermal cycles. The model is applied to construct microstructure maps for different welding procedures including single and dual torch welding. Further, a phase field model approach is proposed for a detailed description of the spatial microstructure gradients throughout the HAZ. An outlook is provided for integrating the microstructure model with a temperature and property model.

P-38: Model Uncertainty Quantification of Calibration Data Volume in bcc Fe Crystal Plasticity: *Aaron Tallman*[1]; Laura Swiler[2]; Yan Wang[1]; David McDowell[1]; [1]Georgia Institute of Technology; [2]Sandia National Laboratories

Scientific models and simulations generally have structure that is bound to hypotheses. The degree to which these hypotheses are testable is an important concern in the endeavor to improve upon existing models. A description of the testability of model structure is approached by examining the process of model calibration. A Crystal Plasticity model is used to simulate the temperature dependent single crystal yielding of bcc Fe. The model is calibrated with experimental data on the orientation and temperature dependent single crystal yield strength of bcc Fe. The calibration is performed incrementally. Separately, the model is calibrated with pseudodata generated from one calibration of the same model. In both calibrations, the model form uncertainty is described using surrogate models to interpolate the sum of squared errors (SSE) across calibration parameter space. The variation in SSE as data is incrementally included is used to inform decisions on the data requirements of the model.

P-39: Modeling AC Electrical Conductivity of Polymer Nanocomposites: *Pouyan Karimi*[1]; Sohan Kale[1]; Iwona Jasiuk[1]; Martin Ostoja-Starzewski[1]; [1]University of Illinois at Urbana-Champaign

Polymer nanocomposites have emerged as an important class of materials finding a wide range of conductive, semiconductive, and static dissipative applications. The complex ac impedance of carbon nanocomposites, taking into account the tunneling conductivity between nano-fillers has been studied. Real and imaginary parts of the complex conductivity vs. the frequency and the filler fraction are presented for three-dimensional systems. A code has been developed to investigate the relation between microstructure and frequency-dependent electrical properties of nanocomposites including permittivity and conductivity using RC type simulation analysis. Our work focused on finding the admittance vs. frequency for equivalent circuit. Resistor and capacitor values are deduced from a random microstructure. These results are compared with experimental data obtained on a nanocomposite material composed of electrically conductive fillers dispersed in an insulating matrix, a good agreement was found between the simulated and experimental results. It is evident that this simulation largely succeeds in explaining the experimental data, such as the complex impedance and its frequency dependence. The results for frequency-dependent permittivity and conductivity can be used as an input to calculate the shielding effectiveness of polymer nanocomposites. In addition, we are exploring the possibility to model a strongly heterogeneous material, based on the microstructure, using an improvement of an RC type model by considering a temperature dependence of the conductivity.

P-40: Molecular Dynamics Study of Nanoparticles Sintering in Laser Assisted Deposition Process: *Ji-Hyeon Song*[1]; Sung-Hoon Ahn[2]; Yan Wang[1]; [1]Georgia Institute of Technology; [2]Seoul National University

Understanding the laser effect on sintering is important for particle based additive manufacturing. How temperature and morphology of particles change with laser irradiation is a primary issue determining the quality of deposition results. Yet, they are very difficult to be directly measured by experiments. In this research, the sintering of nanoparticles in a laser assisted deposition process is simulated using molecular dynamics. In this system, nanoparticles at the aerosol state are heated by laser below the melting point. The dynamics of thermal property and morphological change of particles during the sintering are predicted. Interaction between particles and the surrounding environment is simulated. The effects of controllable process parameters such as laser intensity, aerosol pressure, and particle sizes are studied. Process parameters are optimized for the purpose of process planning. Simulations are also compared with experimental results.

P-41: Multiscale Materials Modeling, 3D Materials Science, Representative Volume Elements and More: Selected Advances and their Relevance to ICME Frameworks: *Dennis Dimiduk*[1]; Mike Groeber[2]; Michael Uchic[2]; [1]BlueQuartz Software, LLC; [2]Air Force Research Laboratory

Research on multiscale materials modeling has proceeded in earnest for about 40 years. Further, 3-dimensional materials science methods (3d-MSE) have been emerging for nearly two decades. Yet, there is little penetration of the tools, techniques and methods into industrial design, manufacturing and materials engineering. Here we selectively examine materials and structures multiscale modeling and 3d-MSE development from the aspects of i) experimental techniques/instruments; ii) data processing and segmentation; iii) data analysis, quantification and representation; iv) 3d structures and model building; and, v) predictive simulations. These examinations are conducted across scales of hierarchical materials structure using selected examples. From the assessment we suggest that more unified and holistic approaches are needed, cutting across engineering disciplines, to achieve widespread use of these methods within the design-materials and manufacturing enterprise. We also conclude that costs and the slow-to-develop knowledge base of skilled practitioners also present obstacles to adoption.

P-42: Multiscale Uncertainty Propagation in Molecular Dynamics: *Anh Tran*[1]; Yan Wang[1]; [1]Georgia Institute of Technology

Modeling the propagation of uncertainty with respect to time in molecular dynamics (MD) simulation is important to understand the system behavior in details. In this work, the evolution of aleatory and epistemic uncertainty associated with thermodyanmics properties as the quantities of interests (QoIs) is modeled at two time scales. At the short time scale, the probability density distributions (PDFs) for QoIs are evolved at each step of MD simulation. At the long time scale, a stochastic dynamics model is proposed to propagate PDFs more efficiently with an upscaling scheme. Examples of viscosity and thermoconductivity based on Green-Kubo approach are demonstrated.

P-43: Nano Simulation Study of Mechanical Property Parameter for Microstructure-based Multiscale Simulation: *Kazuki Mori*[1]; Mototeru Oba[1]; Sukeharu Nomoto[1]; Akinori Yamanaka[2]; [1]ITOCHU Techno-Solutions Corporation; [2]Tokyo University of Agriculture and Technology

We have proposed the microstructure-based multiscale simulation of hot-rolling process of a duplex stainless steel using multi-phase-field and finite element methods. In the multiscale simulation, it is key to use accurate elastic constants of the constituent phases in the steel. However, because the elastic constants depend on chemical composition of the steel and temperature, it is difficult to obtain the elastic constants for multicomponent steels from database and databook. In the previous our work [S. Nomoto, et al., Integrating Materials and Manufacturing Innovation, submitted], the elastic constants of the constituent phases in the duplex stainless steel (Fe-Cr-Ni-C alloy) was calculated by first principle calculation and molecular dynamics simulation. The calculated elastic constants were good agreement with experimental ones. However, these results were obtained from 11 configurations of Fe, Cr, and Ni atoms without much considering local dispersion of Cr and Ni atoms. In this study, the elastic constants were calculated from 10000 atomic configurations by molecular dynamics simulation. As a result, the dispersion of the calculated elastic constants showed the Gaussian distribution. The factor of the Gaussian distribution of the elastic constants was revealed by the Radial Distribution Function.

P-44: On the Deformation Mechanisms of Three-Dimensional Core-Shell Nanoporous Metals: Lijie He[1]; Haomin Liu[1]; Bin Ding[1]; *Niaz Abdulrahim*[1]; [1]University of Rochester

Nanoporous (NP) metallic structure shows brittleness under tensile loading despite of its ductile constituent ligaments. the brittleness of the NP structure is mostly attributed to the morphology of one dimensional nanoligaments randomly distributed in a three dimensional network structure. Preliminary experiments have revealed that electroplating a shell on the NP structure can significantly increase the hardness of the system. This study focuses on the effect of adding a shell to both a single ligament and a 3-D NP structure. We investigate topological and morphological parameters including surface and interface effects, ligament and pore sizes, orientation and loading direction, shell-layer thickness and surface chemistry on the overall mechanical behavior of NP structure and determine the corresponding deformation mechanisms. Our goal is to determine how these parameters should be tuned to achieve better ductility in NP metallic structures.

P-45: Ontology Project for Knowledge-driven Optimization for ICME Approach: *Piotr Maciol*[1]; Lukasz Rauch[1]; Andrzej Maciol[1]; [1]AGH-University of Science and Technology

Development of new materials, products and technologies with ICME approach requires challenging computations, controlled by optimization algorithms. One of the possible ways of decreasing of computational time is "knowledge-driven optimization" – an optimization is controlled not only by a numerical algorithm, but also with a Knowledge Based System. This justifies development of a common language, able to cover communication between numerical models without sophisticated translators. There are several formalisms of knowledge description. In general, more strict formalisms lead to more difficult definition of knowledge but higher efficiency of reasoning. The most of reasoning systems are based on first order logic and knowledge defined with Horn clauses (IF-THEN rules). However, transformation of practical knowledge involved in ICME processes onto the form of such clauses is difficult, mainly due to uncertainty and incompleteness of data, structured data (ranged, tabular and others) as well as a large amount of technological knowledge. Furthermore, management of a coherent set of rules is a complex process itself and must be done by knowledge engineer, not domain experts. We present an approach to develop an environment of knowledge management, combining Semantic Web approach, first order logic based reasoning systems, fuzzy sets and fuzzy logic. In our approach the OWL-based ontology is used to define the language of communication between computer programs (including numerical models and databases). Furthermore, the ontology is used to control consistency of knowledge. The exemplary multiscale problem is described, including alternative technological paths. OWL based ontology and rules controlling optimization process are also included.

P-46: Optimization of High Entropy Alloys: *Paul Jablonski*[1]; Michael Gao[1]; John Sears[1]; Jeffrey Hawk[1]; [1]US Department of Energy

High entropy alloys (HEA) have a 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. Traditionally, researchers have relied on a simple calculation to determine this configurational entropy which results in equiatomic compositions. Here an alternate approach is used where CALPHAD method is used to calculate the optimum (highest) entropy for a system of elements. This approach results in a non-equiatomic alloy formulation. In this research we compare the optimized formulations to equiatomic ones for the same system of elements. These alloys are made as large-scale ingots in our laboratory using detailed process control. Our preferred manufacturing approach is to employ induction melting to combine the constituents followed by a computationally optimized homogenization treatment to eliminate the segregation that occurs during solidification. At this point the ingot is prepared for hot working via forging and rolling. The resulting structure is fully wrought and comparable to alloy manufacture on the commercial scale. Alloy design, microstructure, tensile properties and creep behavior will be presented as comparisons between the formulations. A discussion regarding alternative approaches to material fabrication and the impact on resulting properties will also be presented.

P-47: Predicting Mechanical Properties and Material Transient Behavior of a Metastable Austenitic Stainless Steel by a Mechanism-based Simulation Model Considering Prehistory Effects: *Martina Zimmermann*[1]; Philipp-Malte Hilgendorff[2]; Andrei Grigorescu[2]; Claus-Peter Fritzen[2]; Hans-Jürgen Christ[2]; [1]TU Dresden; [2]Universität Siegen

Reliability of components strongly depends on material microstructures which in turn are significantly influenced by manufacturing processes applied. In this respect, metastable austenitic stainless steels are of particular interest, since they allow for an adjustment of the local mechanical properties by taking advantage of the phenomenon of a deformation-induced phase transformation. In the present study experimental analyses on the static&cyclic strength of AISI 304 in different pre-deformed conditions were extended by modelling and simulation approaches. Two-dimensional microstructures consisting of a representative number of grains were modelled using the boundary element

method and plastic deformation within the microstructure was considered by mechanism-based approaches. As such, cyclic plastic deformation in shear bands and deformation-induced martensitic phase transformation were defined and implemented. Simulation results were directly compared to the observed deformation evolution on the real specimen surfaces. Cyclic softening and hardening behavior mirrored by the resonance behavior of the specimens during fatigue testing was compared to the predicted change in damping behavior due to the transient behavior on the basis of the simulation model. Good agreement of results confirms the model assumptions and allowed for assigning certain deformation mechanisms to the specific change of transient resonant behavior. The outcome of the study can be used for future computational materials engineering in two different ways – a mechanism based approach to adjust mechanical properties prior to the design of new forming processes and a basis for structural health monitoring (SHM) techniques measuring vibrations during operation and relating them to the transient material behavior.

P-48: Predicting Processing-Structure-Property Relationships in PAN Based Carbon Fibers Using Molecular Dynamics Simulations: *Saaketh Desai*[1]; Alejandro Strachan[1]; [1]Purdue University

Carbon fibers are an important class of materials, their high tensile strength and stiffness combined with their low density and chemical reactivity enable advanced composites for a wide range of applications. Commercial fibers can approach the modulus of ideal graphite but at the expense of strength and even high-strength fibers (with reduced stiffness) do not surpass 10% of the ideal strength. The development of high-strength and high stiffness fibers could be accelerated if processing-microstructure-property relationships were available; unfortunately these relationships remain empirical and we lack predictive tools. We will present a new molecular model to simulate the carbonization process of PAN based precursors and the development of microstructure in carbon fibers, and the predicted structural features are in agreement with experiments. We then characterize the mechanical properties of the predicted atomistic models using reactive molecular dynamics. The simulations enable us to extract quantitative processing-structure-property predictions that can provide insight to experimentalists working on the design of next-generation fibers.

P-49: Prediction of Continuous Cooling Trasformation Curves for Steels from Database: *Makoto Watanabe*[1]; Takuya Kadohira[1]; Satoshi Minamoto[1]; Susumu Tsukamoto[1]; Tadashi Kasuya[1]; Junya Inoue[1]; [1]National Institute for Materials Science

Continuous Cooling Transformation (CCT) Curves represent phase transformation behavior depending on cooling rate. Thus CCT diagrams are significantly important to understand microstructure evolution and to estimate mechanical properties of steel welded parts. However, microstructure evolution and phase transformation behavior of steels is quite complicate, and predictions of CCT curves are still a challenging research subject. In National Institute for Materials Science (NIMS) in Japan, we have the database of steel CCT curves which has been obtained through reliable and well organized experiments. In this work, several attempts to predict CCT diagrams have been performed by utilizing the NIMS database and basic machine learning techniques and the summarized results will be presented in the presentation. Although there are still large errors between the predication and the experimental data for some steels, it has demonstrated high possibility to predict CCT curves from the reliable data base and appropriate analysis techniques.

P-50: Predictive Simulations of Polymers: *Lorena Alzate Vargas*[1]; Chunyu Li[1]; Michael Fortunato[2]; Alejandro Strachan[1]; Coray Colina[2]; [1]Purdue University; [2]University of Florida

Applications of polymers have spread into numerous industrial and technological fields. Current optimization and certification of polymer is mainly based on experimental tests leading to lengthy and costly cycles. Predictive simulations have the potential to contribute to a more effective approach to material design and certification. In this talk, we will discuss how to conduct molecular dynamics simulations to predict polymer properties. Detailed procedures from building polymer chains or monomers from the cloud to the polymerization of different systems will be presented. The effects of molecular force field, atomic charge assignment, annealing and deformation conditions on thermo-mechanical properties of these polymers will also be systematically analyzed, specifically we focus in the prediction of glass transition temperature for PMMA structures and the effect of the building procedure implemented with Polymer Modeler and PySIMM, the forcefield: pcff and DREIDING, in which we have noticed higher predictions of Tg (about 40 K) for the second generation forcefield pcff, and the molecular structure obtaining that systems with large chains show higher predicted values compared to small chains. We are expecting that atomistic simulations can provide quantitative predictions for a wide range of properties for polymers.

P-52: Simulation Analysis of Co-continuous Ceramic Composite Dynamic Mechanical Performance and Optimization Design: *Hongmei Zhang*[1]; [1]Beijing Institute of Technology

Dynamic mechanical performance of co-continuous SiC3D/Al composites is simulated with a realistic three-dimensional(3D) model which is constructed using the proposed generation-based optimization method in this paper. Then an optimization design of different infill materials, volume fractions and distribution characters is proposed. The influences of infill material, volume fraction and core distribution on the dynamic behavior of composite are investigated systematically. The results indicate that the SiC3D/Al composites have the best dynamic behavior, and the failure stress raises significantly along with the increasing of SiC volume fraction. But in the unloading stage, the composites appear a sustaining compressive capacity when the SiC volume fraction is lower. Remaining mass rate and failure contour are studied to research the failure process. The failure stress is also influenced by the distribution characters significantly, and the composites have an optimum structure when C equals 0.02.

P-53: Statistical Tools for Quantifying Grain Boundary Crystallography-Property Relationships: *Srikanth Patala*[1]; [1]North Carolina State University

Grain boundaries (GBs) influence a wide array of physical properties in polycrystalline materials and play an important role in governing microstructural evolution under extreme environments. While the importance of interfaces is well documented, their properties are among the least understood of all the defect types present in engineering material systems. This is due to the vast configurational space of interfaces, resulting in a diverse range of structures and properties. In this talk, I will introduce a novel computational technique for computing the lowest-energy grain boundary structures in the full crystallographic phase-space (misorientations and boundary-plane orientations) of grain boundaries. This high-throughput simulation technique will be integrated with a Bayesian statistical framework for developing predictive five-parameter grain boundary crystallography-energy functions in an efficient manner. The statistical framework will be presented in the context of fcc metals but may be easily extended to materials systems with bcc and hcp crystal structures. These techniques are expected to play an important role in the analysis of grain boundary crystallography-structure-property relationships as they may be extended to the quantification of complex properties, such as diffusivity, conductivity, corrosion resistance, yield strength and defect-interface interactions.

P-54: Strategies and Scenarios Regarding the Engineering and Management of Diagnosis, Maintenance and Reliability of Oil Pipelines: *Anurag Jha*[1]; Nirmal Singh[1]; [1]ISM DHANBAD

The engineering research & the selection and the management application of the most appropriate diagnostic and maintenance methods for oil pipelines, so that to ensure a high level of reliability and second, the structural integrity assessment of domestic oil pipelines presenting metal loss imperfections and defects or deviation from circularity.It presents the nominal and characteristic quantities of oil pipelines the main factors that determine the behavior under load of oil pipelines materials and the materials used for manufacture, the factors and processes leading to degradation of oil pipelines and appearance of anomalies(imperfections and defects) and also the categories and criteria for classification of typical oil pipelines imperfections and defects,like local deformation,cracks or metal loss.It also analyses the modern methods,procedures and means of diagnostic techniques used for oil pipelines imperfections and defects investigation,detection and identification,with emphasis on nondestructive control type,under continuous in-situ monitoring of specific operation parameters.Includes analysis of all unprovoked and provoked damages occurred in the period between 2000 and 2008 years to a domestic oil pipeline according to various parameters based on entries in the Oil Pipeline Record Sheet and the interpretation of results.The following aspects: the construction and functional features of the existing experimental research stands for the mechanical behavior of pipes with and without anomalies on the tubing and designing an experimental program for determining the bursting pressure of the pipes with metal loss anomalies.

P-55: Study of Transient Behavior of Slag Layer in Bottom Purged Ladle: A CFD Approach: *Vishnu Mantripragada*[1]; Sabita Sarkar[1]; [1]Indian Institute of Technology Madras

Purging of argon gas in the molten metal bath is a process, which is regularly involved in secondary steel making operations. The injected gas imparts momentum to the liquid metal which induces high turbulence in the molten metal and helps in homogenization of the bath composition and temperature, and facilitates the slag-metal interactions. In this study, a computational fluid dynamics (CFD) based numerical investigation is carried out on an argon gas stirred ladle to study the flow and interface behavior in a secondary steel making ladle. A transient, three phase coupled level-set volume of fluid (CLSVOF) model is employed to track the slag-metal, gas-metal and slag-gas interfaces. The transient behavior of slag layer deformation and open eye formation is studied for different slag layer to metal bath height ratios at various argon gas flow rates.

P-56: Tensor Random Fields for Stochastic Mechanics: *Martin Ostoja-Starzewski*[1]; Anatoliy Malyarenko[2]; [1]University of Illinois; [2]Mälardalen University

Given that most material microstructures are randomly heterogeneous and non-deterministic, stochastic methods are required for solution of initial-boundary value problems. These methods involve stochastic partial differential equations (SPDE) followed by stochastic finite elements (SFE), and stochastic finite differences (SFD). To proceed, tensor random fields (TRF) of material properties are always needed as input. Note here that most SFE and SFD models and simulations typically rely on simplistic scalar random field assumptions to represent the TRFs of conductivity and elasticity, which effectively are inconsistent with micromechanics and do not account for possible anisotropies. For example, instead of simulating a 4th-rank stiffness tensor field, conventional SFE in Uncertainty Quantification typically employ a scalar random field of Young's modulus along with a constant Poisson ratio or a random field of two Lamé constants. These observations motivate the thrust of this paper: to review the recently developed techniques for explicit representation and simulation of 2nd- and 4th-rank TRFs with the most generally admissible correlation structures. Our models are wide-sense stationary (i.e. spatially statistically homogeneous) and wide-sense isotropic. The representation of a 2nd-rank (and 4th-rank) TRF involves 5 (resp., 29) scalar functions, which cover all the classes of anisotropy; spectral expansions are also available. The scale-dependent, one- and two-point statistics may be calibrated using the Hill-Mandel homogenization condition.

P-58: The NIST Interatomic Potentials Repository in the Era of the MGI: *Zachary Trautt*[1]; Lucas Hale[1]; Chandler Becker[1]; Yechan Choi[2]; [1]National Institute of Standards and Technology; [2]Montgomery College

The Materials Genome Initiative (MGI) seeks to significantly decrease the cost and time of development of new materials, and atomistic/molecular simulation is one area where there is still significant opportunity. While the NIST Interatomic Potentials Repository (IPR) hosts numerous interatomic potentials (force fields), the IPR is not the only place to obtain interatomic potentials, and it can be confusing to determine where models are located and which ones are most relevant. To help users locate relevant information at NIST and other sites, the focus of the IPR is shifting from primarily storing and publishing developer-submitted potentials to: (i) registering potentials and related resources at other locations to enable greater discovery, (ii) carefully computing material properties, fully documented, to help enable users to select an appropriate potential for their use case, and (iii) creating and sharing high throughput property evaluation tools which can operate on local resources instead of requiring external connectivity. A broad overview is given of current status of this effort and future plans within the project.

P-59: The Thermal-mechanical Coupled Simulation of Refractory High-entropy Alloys (WNbTaMo) Additive Manufacturing by Selective Laser Melting: *Hang Zhang*[1]; [1]Xi'an Jiaotong University

The refractory High-entropy alloy (HEA) has excellent properties, such as heat tolerance, high strength to weight ratio, creep resistance etc., which would be advanced material for high temperature-resistant part with complex structure, such as turbine blade. In the work, the experiment and simulation were used to study the selective laser melting (SLM) process of manufacturing the WTaMoNb refractory HEA sample. Adopting the basic SLM process (power (p)=400 W, and scanning velocity (v)=250 mm/s) obtained, the sample with several layers could be deposited. The microstructure was studied, and the interlaced growth and arrangement of tiny dendritic arms increased the porosity of the formed sample and enlarged the crack tendency. The models of thermal transfer during the SLM were built and used to predict the temperature distribution based on the finite difference (FD) method. The thermal stress and strain were simulated and analysed based on finite element (FE) method by inputting the temperature distribution results. The SLM process was optimized by simulation. The optimized process was verified by experiment result, with which the large height of HEA sample could be fabricated successfully.

P-60: Uncertainty Quantification for ICME of Composites: *Loujaine Mehrez*[1]; Ziad Ghauch[1]; Roger Ghanem[1]; Venkat Aitharaju[2]; William Rodgers[2]; Jacob Fish[3]; Colin McAuliffe[3]; [1]University of Southern California; [2]General Motors Company; [3]Altair Engineering, Inc.

Reliable predictive modeling and design for complex systems made of heterogeneous materials can be achieved through the successful coupling of material modeling tools, uncertainty quantification tools, and assimilation tools of available experimental data at a multitude of scales. This work aims at achieving this objective. It is concerned with the construction of predictive probabilistic constitutive models for composite materials that are inferred from data collected at multiple length scales and which are suitable for both prediction and design purposes. Polynomial chaos expansions are well adapted for such tasks and are used to build multiscale probabilistic constitutive models. Specifically, explicit functional relationships are constructed of the macroscopic constitutive properties of the composites with input quantities from the finer scales. These constructions are (i) incorporated in probabilistic experimental calibration as well as propagation of uncertainties, (ii) used to discover the statistical dependencies among inter-scale or/and intra-scale homogenized properties and input quantities, (iii) used to deduce the sensitivities of constitutive homogenized properties at each scale with the input quantities and also with the homogenized properties from the finer scales, (iv) integrated in the design process of complex materials involving manufacturing process, physical and experimental constraints, and appropriate account of variation given the specific nature of heterogeneous materials and modeling errors. The proposed integrated computational modeling process is demonstrated for the design of non-crimp fiber composites under multiscale and multiphysics constraints associated with damage accumulation and manufacturing.

P-61: Uncertainty Quantification in First Principles based Phase Diagram Calculations: *Liang Tian*[1]; Anirudh Natarajan[2]; Anton Van der Ven[2]; Brian Puchala[1]; [1]University of Michigan; [2]University of California, Santa Barbara

The construction of first principles based alloy phase diagrams via lattice-model Monte Carlo calculations using cluster expansion effective Hamiltonians has become increasingly common place. Calculated phase diagrams are very useful for qualitative understanding and can be very effective in guiding and interpreting experiments, but the uncertainties associated with the predictions are generally poorly quantified. Using the software package CASM (github.com/prisms-center/CASMcode) we have developed robust methods for convergence of Monte Carlo calculations, automated phase transition detection, and automated fitting of free energies. We used these methods, applied to the Mg-Cd binary alloy system, to investigate the uncertainty in the calculated free energies and phase diagram due to density functional theory (DFT) calculation errors, cluster expansion basis set, coefficient fitting method, and Monte Carlo calculation convergence. We consider how these tools and results can be used as part of the solution to the challenge of uncertainty quantification in first principles based phase diagram calculations.

P-62: Using Artificial Neural Networks in Microstructure Evolution Prediction of Two-Phase Titanium Alloys. Integrated Computational Materials Engineering (ICME) Approach on the Base of Deform 2D/3D Software: *Anton Ektov*[1]; J.H. Kim[2]; [1]VSMPO-AVISMA Corp.; [2]Hanbat National University

The microstructural evolution of titanium alloys under isothermal and non-isothermal hot forging conditions was predicted using multilayer-multineuron artificial neural networks with feed-forward and back-propagation technique (FFBP ANN). All models were incorporated into finite element (FE) simulation software (DEFORM-3D). A representable Ti-database of properties was collected during analyses of huge amount of laboratory electronic protocols of mechanical properties. For the period since 2005 year all e-protocols being stored on the corporate in-house server was automatically parsed via VBA macro-coding. Ad-hoc programming techniques was created for automated treatment of unordered and sparse experimental tables of laboratory test data. The input parameters for ANN model were the alloy chemical composition and the various multistage heat-treatment routes, and the output parameter was the Ultimate Tensile Strength (UTS), Reduction of Area (RA), Elongation, Impact Strength and Fracture Tougthness (K1C). The goal of ANN training is to adequately predict mechanical properties of the wrought alpha/betaTi-alloys as a function of heat treatment and alloy chemistry. Resulting ANN models were coupled with the FE simulation (DEFORM-3D) in order to predict the variation of phase volume fraction during isothermal and non-isothermal forging. To validate the predicted results from the models, Ti-6Al-4V alloy was hot-worked at various conditions and then the resulting microstructures were compared with simulated data. Comparisons between model predictions and experimental data indicated that the joined ANN models and self-consistent analytic/pseudo-analytic models are in good agreement with experiment. Integrated Computational Materials Engineering (ICME) approach was created during developing and implementing of ANN.

P-63: Using the MOOSE Framework to Predict the Coevolution of Microstructure and Physical Properties in Materials Under Harsh Conditions: *Michael Tonks*[1]; Daniel Schwen[2]; Pritam Chakraborty[2]; [1]Pennsylvania State University; [2]Idaho National Laboratory

Materials engineering is facilitated when we can predict the physical properties that result in a material from a given microstructure. With this capability, we can design initial microstructures that provide the performance needed for a given application. However, this is complicated in materials under harsh conditions because the microstructure evolves throughout its lifetime, degrading the physical properties. However, computational tools that predict the coevolution of the microstructure and properties can be used to ensure proper performance even during microstructure evolution. In this presentation we summarize the capabilities of the Multiphysics Object Oriented Simulation Environment (MOOSE) for modeling the coevolution of microstructure and properties.

INDEX

T

U

V

W

X

Y

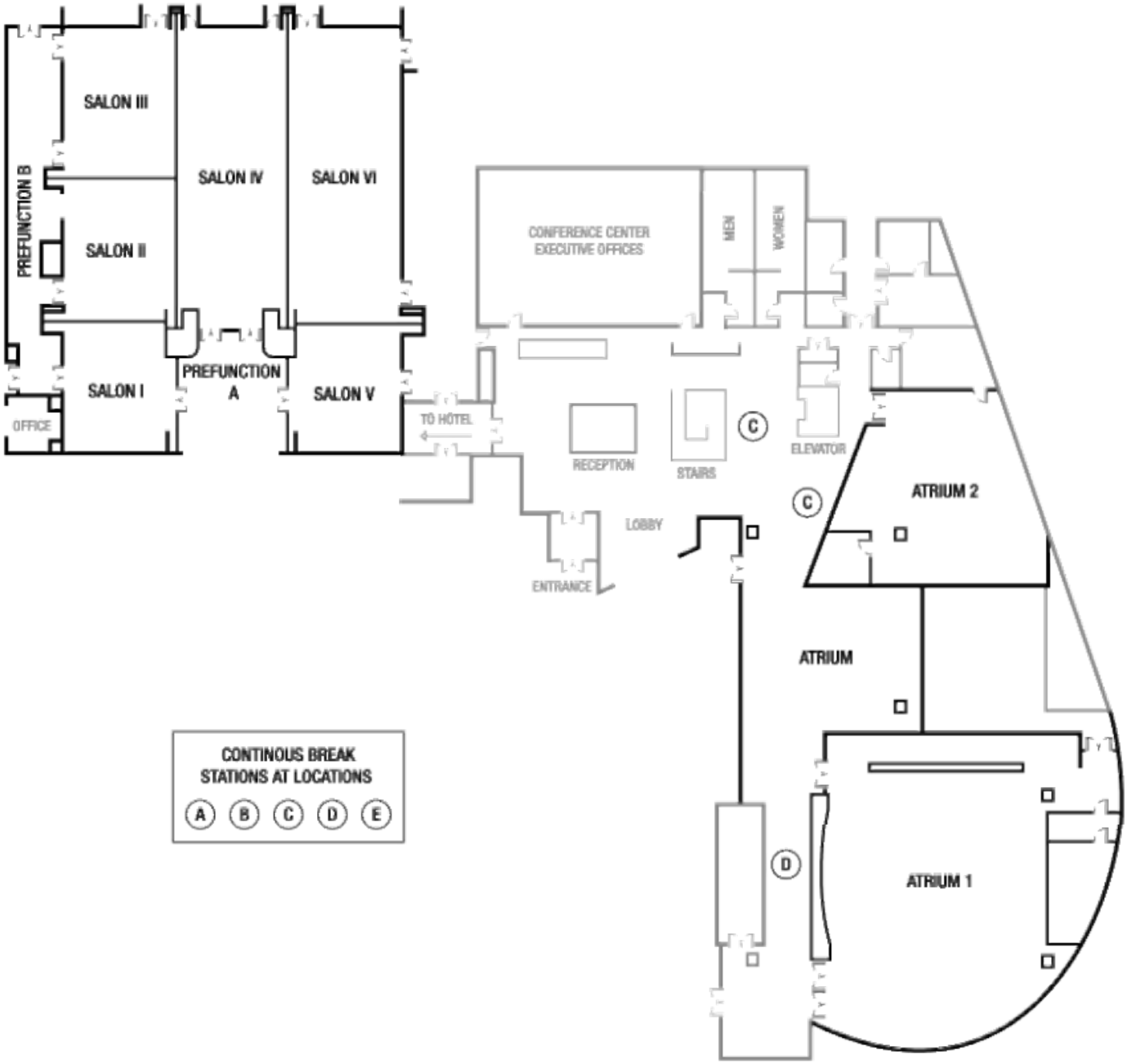
Z

NOTES

NOTES

NOTES

CONFERENCE CENTER
1ST LEVEL



TMS 2018
147th Annual Meeting & Exhibition

THE WORLD COMES HERE.
March 11–15, 2018
Phoenix, Arizona, USA

NOW ACCEPTING ABSTRACTS!

ABSTRACTS WANTED FOR:

More than 80 symposia covering specialized areas within the broader minerals, metals, and materials science and engineering disciplines

CDSM 2018
COMPUTATIONAL DESIGN AND SIMULATION OF MATERIALS

The 2nd International Conference on Computational Design and Simulation of Materials
Jointly organized by the Chinese Society for Metals and TMS, co-located with TMS2018

A Selection of New Symposia

FEMS
TMS
The Minerals, Metals & Materials Society

Organized by the Federation of European Materials Societies (FEMS) and TMS, presented as part of the TMS2018 technical program

SUBMIT YOUR ABSTRACT TODAY!

Submission Deadline: July 1, 2017
www.tms.org/TMS2018