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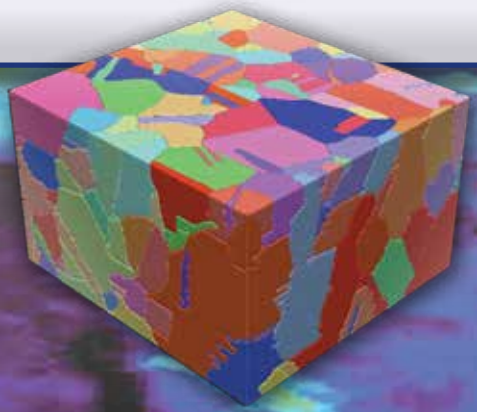
PRELIMINARY TECHNICAL PROGRAM

The content in this preliminary technical program was generated on May 28. However, changes are still being implemented for the final technical program. Please refer to the online session sheets for the most up-to-date information.



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ICME 2019 — ICME Across the Globe

Monday AM
July 22, 2019

Room: White River F
Location: JW Marriott Indianapolis

Session Chair: Charles Fisher, Naval Surface Warfare Center - Carderock

8:00 AM Plenary
The Deep Connections between ICME, MGI, and AI: *James Warren*[1]; [1]National Institute of Standards and Technology
The team that first convened in 2010 to write the founding white paper for the Materials Genome Initiative (MGI) built heavily upon the National Research Council's 2008 ICME report. The report, and a number of it's acknowledged predecessors, allowed for a significant broadening of the engineering impact of the proposed initiative while still preserving the science that is essential to knowledge-based predictive models. Here I will explore the above, how data infrastructures underly the best implementations of these approaches, and how AI is moving these ideas towards a next generation of MGI-inspired research and development.

8:40 AM Plenary
Materials of Tomorrow - The Design Approach: *Annika Borgenstam*[1]; [1]Department of Materials Science and Engineering, KTH Royal Institute of Technology
To accelerate the design of new materials using an ICME approach theoretical as well as experimental tools are needed. In the research center Hero-m 2 Innovation tools for the design of high strength steels, stainless steels, cemented carbides and powder based materials are being developed. Modelling achievements of phase transformation and mechanical properties as well as an improved understanding of the microstructural evolution will be highlighted.

9:20 AM Plenary
Progress in Materials Genome Engineering in China: *Yanjing Su*[1]; Yu Yan[1]; Dawei Zhang[1]; Lijie Qiao[1]; Xuanhui Qu[1]; [1]Beijing Advanced Innovation Center for Materials Genome Engineering, University of Science and Technology Beijing
Materials Genome Engineering (MGE) has been recognized by material scientists and engineers worldwide and it is believed to be a leading technology in the field of materials. Since 2016, China has implemented the National Key R&D Program of the MGE. Great progresses have been made and the advances of the MGE have gradually shown. In this talk, we aim to introduce the progress of the MGE in China, which includes the principles of the MGE, the infrastructure construction, and the advances in the high throughput testing technologies, high throughput calculation software, and materials big data techniques. As well as the application of the MGE technology in the R&D of new materials, such as high temperature alloys and high entropy alloys.

10:00 AM Break

ICME 2019 — Application: Material Design & Alloy Modification I

Monday AM
July 22, 2019

Room: White River I-J
Location: JW Marriott Indianapolis

Session Chair: Danielle Cote, Worcester Polytechnic Institute

10:30 AM Invited
Designing Corrosion Resistant Magnesium Alloys Using ICME Approaches: *Junsheng Wang*[1]; Chi Zhang[1]; Xin Li[1]; [1]Beijing Institute of Technology
Corrosion is a notorious problem for magnesium alloys, limiting their structural applications for many industries. Here, we show how to build an effective Integrated Computational Materials Engineering (ICME) tool to design new chemical compositions and processing conditions avoiding the catastrophic failure of structural components. In addition, the experimental results on the corrosion resistant will also be presented together with ICME predictions, demonstrating the predictive power of ICME approaches.

10:50 AM
Alloy Hunting with Bayesian Optimization: *Matthew Barnett*[1]; [1]Deakin University
The present talk presents an alloy hunt in multi-component space with the aid of Bayesian optimization coupled with a thermodynamic material database (Theromocalc). The search is kept on track via rapid additively manufactured (blown powder) test pieces that are subjected to x-ray diffraction, hardness and scratch testing. The hunt is restricted to compositions that crystallize in the fcc phase. It is shown that Bayesian optimization used in this manner permits one to efficiently explore very broad regions of composition space allowing the discovery of multiple compositions and the mapping of promising regions.

11:10 AM
ICME Design of Advanced Lightweight Steel: *Jiayi Yan*[1]; [1]QuesTek Europe AB
High-aluminum lightweight steel is a new strategy for lighter automotive vehicles and structural components, potentially operative in synergy with existing approaches for improved mechanical properties. However, high-Al steel is still at a low TRL, facing challenges in processing and microstructural control as well as a lack of knowledge. Compared to trial-and-error optimization, ICME materials design approach can accelerate TRL promotion. We present an ICME materials design practice for high-performance ferritic high-Al lightweight steel using best available computational tools and databases. Key links of the processing-structure-properties-performance chain are represented by quantitative models. A first-iteration design material is suggested. We show the potentials of improving mechanical properties and methods to mitigate some known problems, identify factors which limit further design iterations, and suggest directions for future research and development.

11:30 AM
Role of First-principles Calculations in Multiscale Modelling Approach for the Design of Nickel Base Superalloys: *Kaushlendra Kumar*[1]; R. Sankarasubramanian[1]; Umesh Waghmare[2]; [1]DMRL; [2]JNCASR
Superior structural properties of Ni base superalloys are primarily governed by the size, morphology and spatial distribution of γ' precipitates in γ matrix. Designing newer alloys with improved properties requires knowledge of parameters such as lattice misfit, stacking fault energies and elastic moduli as they have a direct bearing on the structure and hence properties. First-principles based density functional theory calculations are employed to quantify the above parameters as a function of alloying elements from 3d, 4d and 5d series transition metals. Their use in higher length scale simulations such as phase-field simulations for morphological evolution, and dislocation dynamics simulations to analyse dislocation interactions as well as analytical evaluation of critical resolved shear stress will be discussed. This approach would provide a rationale for the selection of alloying elements for the design of superalloys with specific properties.

11:50 AM
Design of Ultra-high Strength Stainless Steel by Physical Metallurgy Guided Machine Learning: Chunguang Shen[1]; *Chenchong Wang*[1]; Wei Xu[2]; [1]Northeastern University; [2]Northeastern University, Delft University of Technology
As material research and development entered the big-data era, efficient machine learning (ML) algorithms started to play an important role. Recently, various advanced materials were successfully developed in such manner. However, most of those development based on ML could be considered as a mathematical processing and very litter physical metallurgy guidance was involved in the process, which could inhibit the efficiency of ML. To address this challenge, a novel ML model guided by physical metallurgy was developed. In this model, intermediate physical parameters based on composition and processing parameters were introduced and added to dataset for the ML process. New alloys with relatively lower alloying were designed combining the physical metallurgy guided ML and genetic algorithm, which were experimentally validated with better mechanical properties than the database optimum. Finally, advantages of introducing physical metallurgy principles to the ML were systematically discussed.

ICME 2019 — ICME-based Design Tools I

Monday AM
July 22, 2019

Room: White River F
Location: JW Marriott Indianapolis

Session Chair: To Be Announced

10:30 AM Invited
Incorporating Computer Vision and Machine Learning into the Materials Analysis Pipeline: *Elizabeth Holm*[1]; Andrew Kitahara[1]; Nan Gao[1]; Bo Lei[1]; Srujana Yarasi[1]; Keith Kozlosky[1]; [1]Carnegie Mellon University
To optimize materials and process design, the outcome material must be evaluated with respect to target properties. For image-based data, such as micrographs, computer vision (CV) and machine learning (ML) combine to numerically encode visual information and use it to make qualitative and quantitative judgments about material properties. Thus, CV/ML analysis is a good candidate for inclusion in the ICME workflow. In this talk, we examine industrial case studies of CV/ML for materials analysis. First, we utilize a large database of labelled inclusions in steel alloys to demonstrate that a convolutional neural network (CNN) can classify inclusions by composition, potentially eliminating costly EDS analyses. Second, for powders used in additive manufacturing (AM), we apply CV/ML to characterize individual particles and cluster them by type; we use this baseline to correlate with properties. In both cases, we discuss method selection, limitations, and data requirements for implementing CV/ML in the ICME workflow.

10:50 AM
A Machine Learning Approach for Crystal Plasticity Modeling of Ti-7Al Alloy under Uncertainties: *Pinar Acar*[1]; [1]Virginia Tech University
A two-step stochastic optimization is studied to identify the crystal plasticity (CP) parameters of Ti-7Al alloy. Ti-7Al is an attractive material owing to its superior mechanical properties under large deformations. However, the slip system parameters that are required to understand the CP features are not fully explored. Moreover, the variations in the experimental data impact deterministic solutions. Thus, the realization of the CP model is performed by modeling the uncertainties. First, the possible ranges of the parameters are identified with an inverse problem by utilizing experimental tensile stress-strain curves. Next, the optimization is performed within the new parameter ranges using the compression test EBSD data. A machine learning approach based on Artificial Neural Network is integrated into numerical optimization to achieve the CP model that best mimics the experiments. The findings show that the stochastic solution differs from the available parameters in the literature which are found with deterministic models.

11:10 AM
Deep Materials Informatics: Illustrative Applications of Deep Learning in Materials Science: *Ankit Agrawal*[1]; Alok Choudhary[1]; [1]Northwestern University
The growing application of data-driven analytics in materials science has led to the rise and popularity of the relatively new field of materials informatics. Within the arena of data analytics, in recent years deep learning has emerged as a game-changing technique, which has enabled numerous real-world applications such as self-driving cars. In this talk, I would present some of our recent works at the intersection of deep learning and materials informatics, for exploring processing-structure-property-performance (PSPP) linkages in materials. Illustrative examples include learning the chemistry of materials using only elemental composition, learning multiscale homogenization and localization linkages in high-contrast composites, deep adversarial learning for microstructure design, deep learning for EBSD indexing, and deep transfer learning for crack detection. The increasingly availability of materials databases and big data in general, along with groundbreaking advances in data science approaches offers lot of promise to accelerate the discovery, design, and deployment of next-generation materials.

11:30 AM
Machine Learning-aided Auto-calibration of Phase Field Model for Additive Manufacturing: *Soumalya Sarkar*[1]; Matt Lynch[1]; Ranadip Acharya[1]; [1]United Technology Research Center
Modeling of microstructure in additive manufacturing is growing increasingly important. Energy minimization approaches such as phase field are widely used to predict evolution of dendritic microstructure as a function of material chemistry (concentration) and thermal field. The necessity of sub-micron scale grid refinement and iterative calibration of multiple parameters for the Ginzburg-Landau equation-based potential function make the deployment of phase field models prohibitively expensive. A machine learning framework based on multi-fidelity surrogate assisted constrained Bayesian optimization is proposed for automated calibration. A normalized crispness metric is developed as the calibration objective for the transient problem to ensure sufficient penalty for diffuse interface and concentration deviation. The proposed approach is shown to be capable of reducing the calibration effort from 100s of manual iterations to 10s of iterations as well as able to produce comparable solidification using a 2.5X coarser grid.

11:50 AM
The PRISMS Framework: An Integrated Open-source Multi-scale Capability for Accelerated Predictive Materials Science: *John Allison*[1]; [1]University of Michigan
The Center for PRedictive Integrated Structural Materials Science (PRISMS) is creating a unique framework for accelerated predictive materials science and 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. Specific modules include statistical mechanics, phase field and crystal plasticity simulation codes. The second is The Materials Commons, a knowledge repository and virtual collaboration space for archiving and disseminating information. 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. This talk will review the Center's progress, plans and opportunities for collaboration.

ICME 2019 — Microstructure Evolution and Analysis I

Monday AM
July 22, 2019

Room: White River G-H
Location: JW Marriott Indianapolis

Session Chair: To Be Announced

10:30 AM Invited
Integrating Automated Computational Materials Engineering Workflows for Microstructure-scale Property Assessments in Engineering Design in Manufacturing: *Dennis Dimiduk*[1]; Marcus Hanwell[2]; Robert O'Bara[2]; Sean Donegan[3]; Michael Groeber[4]; Glen Hansen[5]; Thomas Corona[2]; Michael Jackson[6]; [1]BlueQuartz Software LLC; [2]Kitware, Inc.; [3]Air Force research Laboratory; [4]The Ohio State University; [5]Sandia National Laboratories; [6]BlueQuartz Software, LLC
Frameworks for integrating materials performance assessments at the microstructure scale, within engineering design or manufacturing simulation, are under-developed. Our research demonstrated an open-source framework for multiscale simulations using two case studies. Case I assessed equiaxed grain growth during heat treatment within zones of an engine disk forging, by integrating output from DEFORM forging simulations, with DREAM.3D analyses, thermal modeling from the Albany FEM code, and grain-growth simulations using SPPARKS. Case II examined effects of microtextured regions within a titanium engine rotor. This Case integrated microstructure building from DREAM.3D with multiscale stress solutions from Albany, to examine locally-enhanced stresses from the microtexture. Multiscale geometries and meshes for both Cases were developed within the Computational Model Builder (CMB) project. The ICME framework is composed of a Python-based server component built on the Girder project and executed via the Girder Worker feature. Command-line tools permit automated execution. The ICME challenge, developed workflows, and results from these Cases will be presented.

10:50 AM

AixViPMaP® - An Operational Platform for Microstructure Modelling Workflows: Lukas Koschmieder[1]; Stephan Hojda[2]; Markus Apel[3]; Ralph Altenfeld[3]; Youness Bami[3]; Christian Haase[1]; Hamidreza Farivar[1]; Mingxuan Lin[1]; Aditya Vuppala[2]; Gerhard Hirt[2]; *Georg Schmitz*[3]; [1]IEHK RWTH Aachen; [2]IBF RWTH Aachen; [3]Access E V

Modern materials engineering tasks require the consideration of a variety of phenomena eventually determining the microstructure and the properties of a material. These challenges require a modular, configurable system of simulation tools and a framework allowing orchestrating workflows in such multi-model simulation scenarios. Focus of this presentation is the Aachen ("Aix") Virtual Platform for Materials Processing AixViPMaP® which allows a modular combination of some major academic and commercial software tools for the description of microstructures and their evolution by continuum models. It pragmatically draws on HDF5 type datasets as the major means for the communication amongst different microstructure models . Its operation will be demonstrated for three different workflows and an outlook on the benefits of such simulation platforms is providedThe research leading to these results has been performed within the MarketPlace project and has received funding from the European Unions Horizon2020 program under grant agreement n° 760173

11:10 AM

Micromechanics Driven Design of Martensitic Steel Microstructures: *Anssi Laukkanen*[1]; Matti Lindroos[1]; Tom Andersson[1]; [1]VTT Technical Research Center of Finland

Martensitic microstructures are common in modern high strength steel grades. In current work a micromechanics driven ICME workflow was introduced to design wear resistant martensitic high strength steel microstructures. Microstructure based wear model was adopted to first investigate failure mechanisms of martensitic steels under contact. Second, a toolset enabling the modification of imaging based microstructures was developed and applied to yield morphologically and orientation wise differing virtual microstructures to study the structure-performance causality with respect to wear resistance. This enabled the identification of microstructural characteristics yielding potential improvement with respect to abrasive wear performance. The most potential candidates were manufactured and experimentally tested in full scale component loading conditions. The use of virtual performance testing and optimizing microstructural morphologies with respect to wear and fatigue resistance resulted in larger than two-fold decrease in wear rate. As such, the ICME designed steel grades significantly exceeded the performance of existing commercial ones.

11:30 AM

Integration of the CASM Statistical Mechanics Software Package with the Materials Commons Collaboration Platform and Information Repository: *Brian Puchala*[1]; Terry Weymouth[1]; Glenn Tarcea[1]; Anton Van der Ven[2]; John Allison[1]; [1]University of Michigan; [2]University of California, Santa Barbara

CASM is an open source statistical mechanics software package that automates the construction and first-prinicples based parameterization of effective Hamilitonians that can be used to calculate finite temperature thermodynamic and kinetic properties of multi-component crystalline materials. In an ICME framework, free energy and kinetic descriptions such as those generated by CASM provide a critical link between the chemical composition design space and macroscopic material properties. To make CASM generated data more easily available for use in materials discovery and design, multi-scale modeling, and materials optimization, we have developed an integration with the Materials Commons collaboration platform. With this tool researchers can store CASM data in the Materials Commons along with complete provenance information for traceability and reproducibility. Once uploaded, CASM results can be shared privately with collaborators for analysis and use in the PRISMS-PF phase-field software package and other continuum methods, or published for use by wider community.

11:50 AM

Multi-scale Computational Models for Predicting Fatigue Crack Nucleation in Metallic Materials: *Somnath Ghosh*[1]; [1]Johns Hopkins University

This talk will introduce a multi-scale computational framework for physics-based modeling of fatigue crack nucleation and evolution, in polycrystalline metallic materials. Titanium alloys will be a specific focus. The talk will begin with methods for generating 3D statistically equivalent representative virtual images and representative volume elements from experiments on material characterization. An experimentally validated crystal plasticity finite element (CPFE) model will be discussed for predicting microstructural deformation under monotonic and cyclic loading. The CPFE simulations will provide a platform for the development of physics-based crack nucleation model that accounts for microstructural inhomogeneity. Accelerated simulations for a large number of cycles leading to fatigue crack nucleation will be accomplished by a wavelet transformation based multi-time scaling (WATMUS) algorithm. Subsequently, the development of parametrically homogenized constitutive models (PHCM) will be discussed for macroscopic analysis. It will conclude with a case study on the necessity of multi-scale models for predicting fatigue crack nucleation.

ICME 2019 — Application: Material Design & Alloy Modification II

Monday PM
July 22, 2019

Room: White River I-J
Location: JW Marriott Indianapolis

Session Chair: Danielle Cote, Worcester Polytechnic Institute

2:00 PM

Modelling Precipitation Kinetics during the Ageing Treatment of Al-Mg-Si-Cu Alloys: *Qiang Du*[1]; [1]Sintef Materials and Chemistry

In Al-Mg-Si (AA6xxx) alloys, the precipitation of hardening and grain boundary particles during ageing treatment are affected by the addition of minor alloying component, Cu. It has been observed with High Resolution TEM the Cu addition leads to the change of the types of particles, which entails dramatic changes in the Al-Mg-Si alloy's thermal stability, mechanical properties and corrosion resistance. In this contribution, we take the modelling approach to rationalize some interesting observations revealed recently with the TEM and SPED microstructure characterization technique. It is expected that the combination of the numerical simulation with the detailed experimental characterization could shed some light on the physical mechanisms during the aging treatment of Al-Mg-Si-Cu alloys.

2:20 PM

ICME Design of a Corrosion Resistant HEA for Harsh Environments: *Pin Lu*[1]; Jiadong Gong[1]; Greg Olson[1]; Tianshu Li[2]; Gerald Frankel[2]; Angela Gerard[3]; Kathleen Quiambao[3]; John Scully[3]; [1]QuesTek Innovations LLC; [2]Ohio State University; [3]University of Virginia

The integrated computational materials engineering approach is inherently suited to explore the vast, multi-dimensional high entropy alloy (HEA) compositional and processing space, and has been adopted in this work, coupled with empiricism, to design highly corrosion resistant HEAs. Using the combination of empirical and computational approaches, several non-equimolar HEA compositions were identified for their predicted ability to form a single-phase structure and to exhibit high corrosion resistance. Phase diagrams and E-pH Pourbaix diagrams for HEAs were calculated by CALPHAD. One of the Ni-rich HEA has been successfully synthesized on the lab-scale and homogenized at 1250°C for 120 hours. Exceedingly high corrosion resistance of the Ni-rich HEA was demonstrated by electrochemical testing, including potentiodynamic polarization and electrochemical impedance spectroscopy, even in harsh acidic solutions. The oxides formed on the HEA surface has been characterized. The successful validation of the computational design efforts with pre-set property goals shows that ICME is suitable for corrosion resistant HEA design, including complex non-equimolar HEAs.

2:40 PM

Development of Enhanced Friction Stir Welding (FSW) Tools Using ICME Approach: *Qiaofu Zhang*[1]; Amit Behera[1]; Rajiv Mishra[2]; Jiadong Gong[1]; Greg Olson[1]; [1]QuesTek Innovations LLC; [2]University of North Texas

The application of friction stir welding (FSW) technologies to steels is significantly limited by the high cost and short lifetime of current tool materials. We combined ICME Processing-Structure-Property-Performance models with the experiments to design a new tool material for FSW on steels with enhanced lifetime at a lower cost. QuesTek applied its computational alloy design methodologies to develop and optimize the binder phase for a WC-based FSW tool material to demonstrate the concept of using ICME tools to design hard-facing materials and metal-matrix composites for FSW. In this effort, two optimized HEA compositions as the binder phase materials for WC have been computationally designed and successfully experimentally fabricated and processed, along with characterization of microstructure and mechanical properties. A mechanical property model for the tool material was developed and calibrated using collected literature data, resulting good agreement between predicted values and independent experimental measurements.

3:00 PM

Design of Ti-alloy by Integrating High Throughput Experiments and Calculations: *Libin Liu*[1]; J-C Zhao[2]; Zhanpeng Jin[1]; Xing Wang[1]; Lilong Zhu[1]; Di Wu[1]; [1]Central South University; [2]Ohio State University

The speed for development of new materials is too slow has been emerging as the bottleneck for the innovation of the manufacturing technology. However, on the one hand, application of the computer and information technology to the materials science and engineering has made it possible for us to estimate the properties for single phases, model the microstructure evolutions, and predict the material properties. On the other hand, in order to verify the calculation results, we should develop and use the high throughput methods. In this talk, we introduce some new progress in materials calculation and high throughput experiments, especially the high throughput determination of the phase diagram, diffusion coefficients, and thermal-physical properties; and the high throughput verification of the response of the materials microstructure and properties to the compositions and heat treatment temperatures. Some preliminary results of development of high strength Ti alloy and Bio-Ti alloy has been introduced.

3:20 PM Break

3:40 PM

Design of a New Ni-base Superalloy for Large-scale Casting via High-throughput CALPHAD Computation: Feng Sun[1]; *Lanting Zhang*[1]; Hong Wang[1]; [1]Shanghai Jiao Tong University

Alloy 718 is currently widely used in casting of large-scale (dimension >1 m) components of complex shape for aircraft engine, which has temperature capacity of 650C. The future development of the component requires the temperature capacity be raised beyond 700C with increased size and reduced wall thickness (< 2 mm). We hereby report our recent progress in developing a new alloy meeting the requirements with emphasis on castability and the temperature capacity matching IN939. A high-throughput computation routine based on JMatPro was established, which is capable of performing automatic computations, data extraction and screening in large quantity. 5,203,515 candidate compositions containing Cr, Al, Ti, Co, Mo, W, Nb and Ni were screened via a two-stage process. Two compositions with higher W content and lower Al+Ti compared with IN939 emerged. Experimental validation of the high temperature strength and creep/rupture life at 815C is now in progress.

4:00 PM

Alloy Development of Multicomponent Co-based Superalloys Using High-throughput Diffusion Multiples and Machine Learning: Wendao Li[1]; Changdong Wei[2]; *Longfei Li*[1]; Stoichko Antonov[1]; Ji-Cheng Zhao[2]; Qiang Feng[1]; [1]University of Science & Technology Beijing; [2]The Ohio State University

The novel γ' strengthened Co-based alloys open up a pathway to a new generation of high-temperature materials. However, the exiting Co-based alloys still cannot meet the requirements for widespread engineering applications and the conventional methods of alloy design have only limited success. An ICME approach combining high-throughput diffusion multiples and machine learning was employed to accelerate the optimization of alloying compositions. The diffusion multiples were used to study the interactive effects of alloying elements on the microstructural stability of multicomponent Co-based model alloys The effects of nine elements (Co, Ni, Cr, Al, W, Ti, Ta, Mo and Nb) were systematically studied. The relationships between the compositional variations and microstructural stabilities were established using machine learning tools, based on the datasets of microstructure from SEM characterization and compositional information from EMPA. This combined approach is very helpful to the development of multicomponent γ' strengthened Co-based superalloys for future engineering applications.

4:20 PM

Plasma Modified C-doped Co3O4 Nanosheets for Oxygen Evolution Reaction Designed by Butler-Volmer and First Principle Calculations: *Aoni Xu*[1]; Chaofang Dong[1]; Decheng Kong[1]; Ruixue Li[1]; Li Wang[1]; Xiaogang Li[1]; [1]University of Science and Technology Beijing

13 kinds of modification methods, all aimed at developing an earth-abundant OER catalyst Co3O4 with heteroatoms doped in three different crystal sites, were designed and evaluated by a series of predictive first principle calculations according to Butler-Volmer (BV) equation. Special attention was focused on modification with carbon element doping, which notably narrowed the band gap, lowered polaron migration barrier, and reduced Gibbs free energy. The selected configuration of the electrocatalyst was accomplished by plasma enhanced chemical vapor deposition with low-energy input to assure the appropriate doping site of carbon atoms. A remarkable catalytic activity of 235 mV overpotential at 10 mAcm-2 for the OER on carbon doped Co3O4 nanosheets demonstrate the rationality and feasibility of theoretical prediction. The theoretical study and calculation prediction proposed here which is also applicable for other catalysts and even other electrochemical reaction would be helpful for designing new material or novel modification methods.

4:40 PM

High Throughput Hot Isostatic Pressing Synthesis Technique for Bulk Multi-component Combinatorial Materials: *Lei Zhao*[1]; Lixia Yang[1]; Man Hu[1]; Bin Liu[2]; Hui Wang[1]; Zaiwang Huang[2]; Xuebin Chen[3]; Haizhou Wang[1]; [1]China Iron & Steel Research Institute Group; [2]Central South University; [3]University of Science & Technology Beijing

We designed a honeycomb array structural sleeve made from Pure Ti by additive manufacturing and used hot isostatic pressing (HIP) method based on powder metallurgy and thermal diffusion theories to prepare a bulk combinatorial material with about 100 different composition. In this paper we synthesized a combinatorial sample with the different ratio of Fe, Co, Cr, Ni, etc. and used different high throughput analyzing methods, such as LIBS, micro-XRF,Full-view-metallography, SEM, micro-XRD and Scanning micro hardness etc., to characterize the distribution of composition, structure and hardness property of this combinatorial material. This research put forward a new High throughput HIP synthesis approach and produces a bulk multi-component combinatorial material. It is efficient for material design, the beneficial elements ratio screening and alloy modification. In the future we will try the high throughput phase diagram study combined with magnetron sputtering method.

ICME 2019 — ICME-based Design Tools II

Monday PM
July 22, 2019

Room: White River F
Location: JW Marriott Indianapolis

Session Chair: B. Purushottham Gautham, Tata Cunsultancy Services

2:00 PM Invited

Integrated Computational Materials Engineering-from Delhi Iron Pillar to Additive Manufacturing: *Deepankar Pal*[1]; [1]ANSYS

Delhi Iron Pillar is one of the first examples of using metallurgical constituents in a meaningful manner that helped it realize an appreciable corrosion resistance for atleast 1600 years of recorded history. The metallurgical concoction was perfected such that the materials information chain for Process(Forge Welding), Microstructure(Misawite), Property(passivation) and Performance(corrosion resistance) was apt for its service life. Unfortunately, the ancient knowledge on chemistry selection for apt performance is not available anymore for modern metallurgical processes such as Additive Manufacturing and Castforging. Traditional alloy chemistries are not helpful as they are not optimized for the complex thermo-mechanical history, cooling rates and thermal gradients leading to opportunities for practical applications of ICME. In light of these challenges, process-specific thermophysical property generation using CALPHAD followed by numerical analysis using tools such as ANSYS Thermal Finite Element, Cellular Automata and Crystal Plasticity based Structural Finite Element Solvers for predictions on materials information chain will be discussed during the talk.

2:20 PM

An Integrated Computational Materials Engineering Framework for Designing Sintered Materials: *Tesfaye Molla*[1]; Graham Schaffer[1]; [1]The University of Melbourne

A low order meta model is presented for efficient design of sintered materials optimized for manufacturability and performance. Development of the design method follows the materials systems approach that integrates processing, structure and property relations during metal injection molding and additive manufacturing. It includes a multi-objective genetic algorithm to optimize the chemical composition and processing parameters to simultaneously improve the sintering response and the resultant properties. Thermodynamic simulations, based on the CALPHAD method, are used to establish microstructural constraints through phase stability at equilibrium and calculate the kinetic parameters that determine the sintering behaviour; and predictive models are used to estimate the mechanical properties. To demonstrate the capability of the method, design exercises for a novel austenitic stainless steel and a bimetallic functionally graded material are presented. We show that new alloys with improved sintering/co-sintering performance can be designed while simultaneously enhancing properties by independently controlling composition and processing parameters.

2:40 PM

Data-driven Molecular Dynamics Model of Laser Heating of Inconel 718 Powder with Experimental Validation: Lingbin Meng[1]; Yi Zhang[1]; Jian Zhang[1]; Tao Sun[2]; Yeon-Gil Jung[3]; *Jing Zhang*[1]; [1]Indiana University-Purdue University Indianapolis; [2]Argonne National Laboratory; [3]Changwon National University

In this work, a Gaussian process (GP) based machine learning (ML) model is integrated to a molecular dynamics (MD) model to simulate the laser heating process of Inconel718 powder, a nickel based super alloy extensively used in aerospace industry. First, the MD model is applied to simulate the sintering process under various powder sizes and laser power densities. Then, the GP based model is used to learn the data from the MD model, and makes predictions under new input processing parameters at a small fraction of the time required by a typical MD simulation. The modeling results are compared with the experimental observation conducted by the X-ray Imaging Group at Advanced Photon Source, Argonne National Laboratory.

3:00 PM

Materials Integration Approach for Creep Damage Prediction of Heat-resistant Steel's Weld Joint: *Masahiko Demura*[1]; Hitoshi Izuno[1]; Masaaki Tabuchi[1]; [1]National Institute for Materials Science

Materials Integration (MI) is a concept to link among the fundamental four elements in materials science and engineering such as process, structure, property, and performance using any kinds of methods including experiment, theory, empirical rule, database, and numerical simulations. In fact, we have developed a system allowing us to build and execute a workflow consisting of computational modules, each of which links between one and the other in the four elements. In this study, we utilized the system to predict the lifetime of weld joints of heat-resistant ferrite steels. The workflow we built included a simulation module for welding process, a coarsening module for heat affected zone, and a finite element analysis module for creep deformation and damage accumulation. The computed results reasonably reproduced the experimental ones, indicating that our workflow would be useful to reduce the number of creep experiments to some extent.

3:20 PM Break

3:40 PM

Materials Genome Tools to Predict Calcium-Magnesium-Alumino-Silicate (CMAS) Interactions on Thermal Barrier Coatings (TBC) and Enable Advanced CMAS-resistant TBC Design: *Changning Niu*[1]; David Poerschke[2]; Weiwei Zhang[3]; Carlos Levi[4]; Dana Frankel[1]; [1]QuesTek Innovations LLC; [2]University of Minnesota; [3]Thermo-Calc Software; [4]University of California Santa Barbara

A novel Django-based web toolkit to predict Calcium-Magnesium-Alumino-Silicate (CMAS) interactions on Thermal Barrier Coatings (TBC) is developed to enable advanced CMAS-resistant TBC design. This web toolkit uses TC-Python APIs released by Thermo-Calc in 2018. Detailed functionalities will be introduced, including database management, intrinsic property calculators for down-selecting candidates, and reactivity predictors (adding TBC to CMAS, varying TBC composition, and varying CMAS composition) for further enhanced CMAS-resistant TBC design.

4:00 PM

A Tool to Generate Representative Grain-resolved Open-cell Foam Models: *Joseph Tucker*[1]; Ashley Spear[2]; [1]Exponent; [2]University of Utah

The development and use cases of an open-source filter/plug-in for DREAM.3D that instantiates synthetic, polycrystalline, metallic foam volumes is presented. The new capability allows both for synthetic grain overlay of X-ray computed tomography data as well as fully synthetic geometry and grains. For the latter, a novel technique using Euclidean distances is used to instantiate the 3D open-cell foam morphology, enabling user control of pore size, ligament cross-section shape, and ligament thickness variability. By integrating this approach into the DREAM.3D architecture, the entire DREAM.3D suite of filters is immediately available; thus, enabling both user control and quantification of grain size, shape, and crystallographic orientation statistics (among other things) as well as meshing algorithms to enable subsequent numerical analysis.

4:20 PM

A Framework to Support the Integrated Design of an Energy Absorbent Foam for Football Helmets: *Tate Fonville*[1]; Anand Nellippallil[1]; Mark Horstemeyer[2]; Farrokh Mistree[3]; Janet Allen[3]; [1]Mississippi State University; [2]Liberty University; [3]Systems Realization Laboratory at University of Oklahoma

In this paper, we describe a computational framework for the integrated design of a foam liner to improve the safety of modern American football helmets. Preliminary simulations show our baseline helmet design can dissipate up to 70% of the impact energy where the foam liner alone dissipates 99% of that energy. Therefore, we focus on the integrated design of the polyurethane foam to improve energy dissipation for the overall helmet system. Our baseline foam liner is a viscoelastic, anisotropic open-cell, and polyurethane foam with a thin thermoplastic polyurethane (TPU) film enclosure. We present a computational framework to design the foam liner, with respect to the helmet system, considering two primary variables, namely the liner depth and TPU film thickness. In this paper, we cover the computational framework, analysis, and design space exploration of the material properties of the baseline polyurethane foam and TPU film at the structural scale

4:40 PM

Prediction of Creep Rupture Time for Steels Using Gradient Tree Boosting: *Junya Sakurai*[1]; Junya Inoue[2]; Masayoshi Yamazaki[3]; Masaaki Tabuchi[3]; Masahiko Demura[3]; [1]The University of Tokyo; [2]The University of Tokyo; National Institute for Materials Science; [3]National Institute for Materials Science

The creep test costs long time and is expensive. It is desired to predict the creep rupture time from experimental database. NIMS Creep database contains materials compositions, creep test conditions and rupture time, and the other related properties such as 0.2% proof- and tensile- stresses. This multidimensional variable space is expected to consist of many regions differing in mechanisms, which complexity leads to the difficulty in prediction. In this study, we applied XGBoost, which is an implementation for gradient tree boosting, to achieve precise prediction in a whole variable space for ferrite-base heat-resistant steels. The gradient tree boosting is an effective ensemble learning method using decision trees so that it can perform non-linear regression by dividing the variable space by rules. The resultant predictor showed an excellent performance that the predicted value is within 0.5-2 times of experimental one for test data that were not used for learning.

ICME 2019 — Microstructure Evolution and Analysis II

Monday PM
July 22, 2019

Room: White River G-H
Location: JW Marriott Indianapolis

Session Chair: Georg Schmitz, Access E V

2:00 PM

PRISMS-Plasticity Crystal Plasticity Finite Element Software: *Mohammadreza Yaghoobi*[1]; Sriram Ganesan[1]; Srihari Sundar[1]; Aaditya Lakshmanan[1]; John Allison[1]; Veera Sundararaghavan[1]; [1]University of Michigan

An open source parallel 3-D crystal plasticity finite element (CPFE) software package PRISMS-Plasticity is presented here as a part of PRISMS integrated computational materials engineering (ICME) framework. A highly efficient rate-independent crystal plasticity algorithm is implemented along with developing a new algorithmic tangent modulus. Additionally, a twin activation mechanism is incorporated into the framework based on a Gauss integration point sensitive scheme. Next, the integration of the PRISMS-Plasticity software with experimental characterization techniques such as EBSD and synchrotron X-ray diffraction using available open source software packages of DREAM.3D and Neper is elaborated. The integration of the PRISMS-Plasticity software with the information repository of Materials Commons is also presented. The parallel performance of the software is then investigated. Various examples of polycrystalline metals with different crystal structures of FCC, BCC, and HCP are presented to show the capability of the software to efficiently handle the corresponding problems.

2:20 PM

Modelling the High Temperature Deformation of Superalloys as Emergent Behaviour: *James Little*[1]; Hector Basoalto[1]; [1]University of Birmingham

A field dislocation mechanics (FDM) model is proposed to study slip-induced heterogeneous deformation in Gamma Prime strengthened nickel-based superalloys. The proposed framework accounts for elastic interactions between dislocations, which are included in the evolution equation for the dislocation field and implemented within a finite element model. The development of localised slip bands is simulated for a single crystal representative of a nickel-based superalloy loaded in simple shear, with second-phase particles presenting discrete obstructions to plastic slip. Flow stress responses and elastic-plastic domain back stresses are predicted at temperature for a range of unimodal and bimodal particle dispersions, as well as for the matrix-only case. Experimentally observed trends for precipitate strengthening are recreated numerically. The effect of impenetrable domain boundaries on slip evolution is also investigated, with numerical simulations predicting an inverse square-root dependence of yield stress on the size of the domain, recreating the Hall-Petch response as emergent behaviour.

2:40 PM

An Amplitude Expansion of the Phase-field Crystal Model with Grain Rotation in Full Range and Adaptive Mesh Refinement: *Matjaž Bercic*[1]; Goran Kugler[1]; [1]University of Ljubljana, NTF

An improvement of the amplitude expansion of the Phase-Field crystal model is presented (APFC), enabling the application of adaptive mesh refinement techniques using the Cartesian representation of the amplitude equations. The number of computational nodes scales in proportion with the length of the grain boundaries. The improvement is based on an auxiliary local rotation field which can also be used to enable modelling of grains in a full range of rotations without effects of an unphysical grain boundary. We present the implementation of the modeland calculated energies of symmetric tilt grain boundaries in a model parameterized to match graphene. The results closely match previously published results without effects of an unphysical grain boundary. The APFC model is employed to model dynamically rotating grains through a full range of rotations and compared to results obtained with a Phase-Field crystal model. No effects of an unphysical grain boundary are found.

3:00 PM

Developing a Combinatorial Modeling Approach to Multiscale Modeling and Predictions for High Entropy Alloy Design: *Pratik Dholabhai*[1]; Yongfeng Zhang[2]; Jeffery Aguiar[2]; [1]Rochester of Institute of Technology; [2]Idaho National Laboratory

Current engineering materials qualification involves a series of time-intensive steps and testing cycles. These suffer from an ineffective early down-selection, requiring additional testing and qualification. Combinatorial material modeling has emerged as a viable path to rapidly predict and shorten the list of materials candidates by as much as 50% based on desired material outcomes, such as high thermal conductivities or mechanical strengths. However, few inroads have been made for the development of a rapid process for nuclear or high-temperature structural alloys. In this presentation we will present a combinatorial modeling methodology seldom used to develop high-entropy alloys (i.e., as a proof-of-principle demonstration for a new class of alloys), leveraging fundamental atomic to micron scale information and large-data analysis tools. The approach to readily apply deep, recursive, and transfer learning approaches to organize, classify, and screen candidate materials into new classes of materials will be presented in detail.

3:20 PM Break

3:40 PM Invited

Development and Application of a Microstructure-based Approach to Characterize and Model Failure Initiation in Dual-phase Steels: *Ali Ramazani*[1]; [1]Massachusetts Institute of Technology

In this research, a microstructure-based model is developed to characterize and model failure initiation in DP steels using an extended finite element method (XFEM) to simulate martensite cracking on the mesoscale combined with representative volume element (RVE) modeling. A mini tensile test with digital image correlation (DIC) analysis is linked to local SEM analysis to identify the local strain at which failure is initiated. In-situ bending tests in SEM with electron backscatter diffraction (EBSD) measurements before and after the test are carried out to validate that the crack initiates in the martensite islands. Empirical equations for XFEM parameters as functions of local carbon content in martensite are fit to experimental results for laboratory-annealed DP600 steels with varying martensite content. The equations are then shown to predict successfully failure initiation in industrially produced DP steels with various chemistries, strengths and martensite fractions.

4:00 PM

Microstructure Modeling of Metal in Laser Powder Bed Fusion Process Using Combined Computational Fluid Dynamics and Cellular Automata Method: Lingbin Meng[1]; Yi Zhang[1]; *Jing Zhang*[1]; [1]Indiana University-Purdue University Indianapolis

In laser powder bed fusion process, microstructure can be affected by process parameters. The laser scanned metal may contain columnar grain or/and equiaxed grains depending on thermal history in the melt pool. This work presents a method of using numerical method to predict the microstructure of laser powder bed fused metal. The method is composed of two steps. Firstly, a computational fluid dynamics (CFD) model is developed to simulate powder melting and molten metal flow, the temperature and material distribution during the laser scanning process is predicted. Secondly, the result from CFD model is applied to a cellular automata (CA) code to simulate the solidification process. In the CA model, nucleation and growth of individual grains are simulated, grain type (columnar or equiaxed), grain size, and grain orientations are predicted. A parametric study with varying laser scan speed and powder thickness is conducted, and the resulting microstructures are discussed.

4:20 PM

A Benchmark on Modeling of Incremental Forming of Aluminum 7075-O: Jaekwang Shin[1]; Newell Moser[2]; Hyunki Kim[3]; Farhang Pourboghrat[3]; Jian Cao[2]; Alan Taub[1]; Mihaela Banu[1]; [1]University Of Michigan; [2]Northwestern University; [3]Ohio State University

Finite element modeling of the incremental forming is a very useful tool for designing the process of incremental forming. A unified approach is needed as a guidance for simulation of incremental forming, due the complexity of the physical and numerical parameters to be set-up. As a part of Agile R1-1 Project, University of Michigan, Ohio State University and Northwestern University conducted a benchmark of the incremental forming modeling of a cone having the wall angle of 67° has been conducted against experimental realizations. The benchmark includes the following variables: FEM software, the boundary conditions, the algorithm of meshing, yield criterion, the constitutive material model and numerical parameters such as the optimal meshing and scaling factor. The results show a good consensus in the thickness distribution. However, some differences are obtained in prediction of the force caused by the impact of the material model and contact interaction.

4:40 PM

Molecular Level Modeling of Polymer Crystallization: *Tongtong Shen*[1]; Chunyu Li[1]; Alejandro Strachan[1]; [1]School of Materials Engineering, Purdue University

The degree of crystallinity and microstructure in semi-crystalline polymers governs their thermo-physical and mechanical properties and the control of crystallization during manufacturing remains significantly challenging particularly in processes like automated tape and fiber placement due to heterogeneous nucleation sites and fast speeds. Despite significant efforts, we lack predictive tools to understand relationships between the polymer chemistry and the crystallization thermodynamics and kinetics. We will discuss our recent molecular dynamics studies on polyethylene(PE) and polyetherketoneketone(PEKK) crystallization process with extensive simulations of both all-atoms and united-atoms models. Simulations of PE crystal nuclei growth reveal that lateral growth of primary grain results in significant local deformation, with consequent increase of orientation of surrounding amorphous material and resulting in induced nucleation having correlated orientation. We believe this process a key step of spherulites-like structure development. In the case of PEKK, the simulations capture effects of the terephthaloyl/isophthaloyl(T/I) ratio on glass transition temperature and crystallization.

ICME 2019 — Application: Additive Manufacturing I - Microstructure

Tuesday AM
July 23, 2019

Room: White River F
Location: JW Marriott Indianapolis

Session Chair: To Be Announced

8:00 AM Invited
Microstructural Modeling in Laser Powder Bed Fusion (LPBF) Systems: *Anthony Rollett*[1]; Joseph Pauza[1]; Lonnie Smith[1]; P. Chris Pistorius[1]; Joseph Aroh[1]; [1]Department of Mateirals Sciecne and Engineering, Carnegie Mellon University
Although the basics of microstructure formation in solidification of metals is well understood, i.e., growth of <100> dendrites up the temperature gradient, grain structures observed in 3D printed materials are generally complex. Scan or raster patterns that vary between machines and within parts contribute to this complexity. Here we focus on the effect of melt pool shape, which in turn reflects the interaction between the laser light and the powder and underlying metal. High speed videography with synchrotron x-rays has emphasized the near-universal presence of a keyhole thanks to the power density generally exceeding a boiling threshold. This means that the melt pool shape is far different from that of the commonly assumed point source. We describe how such melt pools can be quantified and incorporated into a kinetic Monte Carlo code, sparks, that enables grain microstructure formation to be simulated for multiple tracks, variable hatch spacing etc.

8:20 AM
The Exascale Additive Manufacturing Project (ExaAM): Process Modeling at the Fidelity of the Microstructure: *John Turner*[1]; James Belak[2]; ExaAM Team[3]; [1]UT-Battelle / Oak Ridge National Laboratory; [2]Lawrence Livermore National Laboratory; [3]Exascale Computing Project
The Exascale Computing Project (ECP, https://exascaleproject.org/) is a U.S. Dept. of Energy effort developing hardware, software infrastructure, and applications for computational platforms capable of performing 10^18 floating point operations per second (one "exaop"). The Exascale Additive Manufacturing Project (ExaAM) is one of the applications selected for development of models that would not be possible on even the largest of today's computational systems. In addition to ORNL, partners include Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), the National Institute for Standards and Technology (NIST), as well as key universities.ExaAM is leveraging existing simulation software and developing new capabilities, and we will describe the physics components that comprise our simulation environment and report on progress using highly-resolved melt pool simulations coupled in a nonlinearly consistent fashion to thermomechanics and cellular automata to drive microstructure evolution. Resulting microstructures are used to determine constitutive mechanical property relationships using polycrystal plasticity.

8:40 AM
Local Property Analysis of AM Microstructures: *Robert Carson*[1]; Steven Wopschall[1]; Curt Bronkhorst[2]; Nathan Barton[1]; James Belak[1]; ExaAM Team[1]; [1]Lawrence Livermore National Laboratory; [2]University of Wisconsin
Additive Manufacturing offers the prospect of unique and interesting component designs, including location specific material properties, requiring coupling microstructure development and local property analysis with process simulation. Given the length scales, physical mechanisms, and response characteristics of interest, finite element codes employing crystal-mechanics-based constitutive models are the appropriate computational approach for the microstructure-to-properties analysis. However, no existing code can handle the complexity of AM microstructures or make use of the resources offered on emerging exascale computers. As such, we have created a new code (ExaConstit) based on the MFEM framework. We present property analysis of microstructures generated from Cellular Automata analysis of process simulations and from experimental observations from the AM-Bench project. Comparison will be made with properties of non-AM microstructures. *Work performed under auspices of the U.S. DOE by LLNL under contract DE-AC52-07NA27344, and supported by ECP (17-SC-20-SC), a collaborative effort of U.S. DOE Office of Science and NNSA.

9:00 AM
A Multiscale Framework to Predict the Distribution of Precipitates during Additive Manufacturing of 15-5 PH Stainless Steel: Surya Ardham[1]; Akash Bhattacharjee[1]; Ajaya Jena[1]; Trinath Gaduparthi[1]; BP Gautham[1]; *Gerald Tennyson*[1]; [1]Tata Consultancy Services
Microstructure in additively manufactured components is influenced by the interplay between solutal and thermal gradients, and can be controlled by varying laser power input, hatch distance and scan speed. In this work, a multiscale modeling approach is used to simulate the sum effect of solutal and thermal fields on microstructure evolution in the meltpool of a 15-5 PH stainless steel. Unsteady heat transfer calculations are carried out on a domain consisting of a powder layer spread on top of few laid-out layers. A binary alloy phase-field model, coupled with thermal and solutal transport, is used to simulate microstructure evolution. Thermodynamic properties of the alloy are computed using CALPHAD approach. The layer-scale and the microstructural scale are coupled via thermal boundary conditions derived from heat transfer calculations. Further, solutal distribution and the effect of solutal and thermal gradients on the interdendritic arm spacing and thereby on the precipitate distribution are predicted.

9:20 AM
Modelling Microstructural Evolution in Additively Manufactured 316 Stainless Steel: *Joseph Aroh*[1]; Anthony Rollett[1]; [1]Carnegie Mellon University
Laser powder bed fusion (LPBF) processes introduce rapid and localized solidification which has a characteristic effect on grain growth. The as-built microstructure is also highly sensitive to process parameters such as laser power and scan velocity. The ability to predict and control the microstructure (e.g. grain geometry and orientation) of a printed part is vital to optimizing material properties, and by extension, material behavior. An open source program called SPPARKS simulates the LPBF build process by implementing a Potts model code in a localized layer-by-layer process. Analytical and empirical methods can be embedded into the SPPARKS code to optimize the model for 316 stainless steel. Cross-sectional analysis of melt pool geometries and isothermal grain growth data for 316 will be used to fine-tune these modifications to SPPARKS. Comparisons between the 316 optimized SPPARKS code and printed 316 parts across an array of power-velocity inputs will validate this model.

9:40 AM
Cellular Automata (CA) Modeling of Microstructure Development during Additive Manufacturing Processing*: *Matthew Rolchigo*[1]; Alex Plotkowski[2]; James Belak[1]; ExaAM Team[1]; [1]Lawrence Livermore National Laboratory; [2]Oak Ridge National Laboratory
Alloy microstructure development during the extreme conditions of Additive Manufacturing is multifaceted, depending on local thermal conditions, kinetics and thermodynamics of solidification, and previous layer microstructure. We apply a 3D Cellular Automata (CA) model for as-solidified Inconel, with grain growth based on ternary alloy solidification theory. Several methods for modeling nucleation are introduced, and texture development and the columnar to equiaxed transition are explored. Using a high-fidelity fluid and heat transport model of the AM process (OpenFOAM), complex scan patterns are simulated and predicted thermal conditions are linked to microstructure development and compared to experimental observations from AM-Bench. The scalability of the model to large-scale problems and its use as a component of the exascale ExaAM project are discussed as well. *Work performed under auspices of the U.S. DOE by LLNL under contract DE-AC52-07NA27344, and supported by ECP (17-SC-20-SC), a collaborative effort of U.S. DOE Office of Science and NNSA.

10:00 AM Break

10:30 AM
Prediction of Mechanical Behavior of AM Materials Using Gurson Plasticity: *Yi Zhang*[1]; Mohammad Masoomi[1]; Ali Najafi[1]; [1]ANSYS, Inc.
The linkage between process-structure-property is a challenging task in the recent developments and application of additive manufacturing (AM). Simulation is a useful tool to investigate this relationship, since it can reduce the experimental cost and trial-and-errors. This work presents a simulation framework that predicts mechanical properties with different additive manufacturing process parameters. In this framework, the process parameters are taken into ANSYS Additive Science (a thermal simulation) to predict the AM structures in microscale. The parameters in Gurson plasticity model are obtained from the representative volume element (RVE) analysis based on the simulated AM structures. Finally, the plasticity behavior with varying process parameters is investigated by a simulated tensile test using the Gurson model. Preliminary results show that a lower porosity tends to increase the tensile strength but decrease the elongation.

This framework provides a useful tool for understanding the process dependent mechanical properties, therefore optimizing the AM build process.

10:50 AM
Fatigue Behavior of Additive Manufactured IN718 and Ti-6Al-4V through Coupled Modeling and In Situ Experiments: *Michael Sangid*[1]; [1]Purdue University
The benefits of additive manufacturing have been well documented, but prior to these materials being used in critical applications, the mechanisms for fatigue failure must be identified and the life of these materials must be determined for use in a design context. In this work, the fatigue behavior of selective laser melting IN718 and Ti-6Al-4V is investigated through detailed characterization and modeling efforts. Specifically, in situ loading is used to identify the strain evolution in these materials through high-energy x-ray diffraction and digital image correlation. Simulation-based predictions of material performance, including fatigue crack initiation have been developed as a means of accelerating the insertion of new materials by reducing the associated cost and time for materials development. The fatigue modeling framework is combined with validation and verification efforts of the model's readiness level, in order to build trust in the predictive capabilities of the model.

11:10 AM
Integrated Computational Materials Engineering in Prediction of Thermal and Thermally Motivated Deformation Behavior of Parts Produced using Additive Manufacturing: *Deepankar Pal*[1]; Abdul Khan[1]; Dave Conover[1]; Steve Pilz[1]; Paul Mason[2]; Kaisheng Wu[2]; Adam Hope[2]; [1]ANSYS; [2]Thermocalc
Additive Manufacturing enables fabrication of material microstructures and part geometries at the "energy source" resolution leading to thermomechanical property variations at these length scales. These variations are dependent on the evolving microstructure and back-stresses which are further dependent on solidification rate (R), thermal gradients (G) and residual stresses and can be respectively derived from the thermal and thermally assisted deformation evolutions. To improve the accuracy of the models, it is necessary to predict thermal evolution and part deformation during Additive processing using thermophysical properties obtained as a function of chemistry and solute-drag at the solid-liquid interface enabled using the CALPHAD approach. This approach allows for the full characterization of the thermal and thermally motivated deformation process map as a function of process parameter and powder chemistry variations generally provided by the powder vendors. The process maps mentioned herein along with their experimental validation counterparts will be discussed during this talk.

11:30 AM
Concurrent Build and Melt Pool AM Simulations through Multi-physics Code Coupling*: *Matthew Bement*[1]; Neil Carlson[1]; Neil Hodge[2]; Stuart Slattery[3]; John Turner[3]; [1]Los Alamos National Laboratory; [2]Lawrence Livermore National Laboratory; [3]Oak Ridge National Laboratory
In order to perform melt-pool scan simulations in the extreme conditions of additive manufacturing, a coupled multi-physics thermal/fluid/solid mechanics capability is needed. A LLNL developed thermal mechanics code is used to simulate an AM build on a coarse grid up to a particular point in the build. This thermal mechanics code is then coupled to a LANL developed thermal fluid code to simulate the next few layers of the build on a significantly finer grid for the purpose of enabling melt-pool fluid flow informed prediction of residual stresses. Results will be presented for a representative portion of the NIST AM-Bench 18-01 benchmark problem. *Work supported by ECP (17-SC-20-SC), a collaborative effort of U.S. DOE Office of Science and NNSA.

11:50 AM
Melt Pool Modeling of Laser-powder Bed Fusion Additive Manufacturing Considering Non-spherical Particles: *Xuesong Gao*[1]; Wei Zhang[1]; Guilherme Faria[1]; Kamalnath Kadirvel[1]; Antonio Ramirez[1]; Yunzhi Wang[1]; [1]The Ohio State University
Metal powder particles used for additive manufacturing, commonly produced by gas atomization, tend to have spherical shapes but with important non-sphericities such as satellites and joined particles. Currently, the quantitative understanding of the effect of non-sphericities on melt pool behavior is limited. This study extended existing particle-scale models for laser-powder bed fusion to consider non-spherical particles. Specifically, satellites and joined particles were modeled by "attaching" several spherical particles together to form clumps. The packing of spherical and non-spherical particles on powder bed was simulated using discrete element method. The calculated packing information was then mapped into a heat transfer and fluid flow model, which took into account various important phenomena including interactions between laser beam and individual particles, Marangoni shear stress, free surface evolution, keyhole dynamics, and laser multiple reflections. Simulation results showed that the existence of non-spherical particles reduced the packing density and promoted the formation of porosity defects.

ICME 2019 — Material Databases and Platforms

Tuesday AM
July 23, 2019

Room: White River G-H
Location: JW Marriott Indianapolis

Session Chair: Emine Gulsoy, Northwestern University

8:00 AM Invited
Center for Hierarchical Materials Design: Workforce Training and Continuing Education for Industry: *Emine Gulsoy*[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. CHiMaD's outreach program aims to actively engage industrial stakeholders in both continued design training and efforts in community building and best practices. CHiMaD is also committed to the training of the next generation workforce to be integrated into industry. The presentation will provide an overview of CHiMaD's design training strategy both for current and continuing ICME and design education, as well as points of and opportunities for industry involvement.

8:20 AM
Online Simulation-powered Educational Resources for ICME: Alejandro Strachan[1]; *Tanya Faltens*[1]; [1]Purdue University
Simulations tools have powerful pedagogical potential in ICME that has yet to be fully explored. We will describe a set of online simulation tools and associated learning modules that have been designed to help students explore important concepts in materials science through interactive activities that use simulations to provide new insight into materials behavior. The learning modules cover a range of topics including plastic deformation in metals, the effect of doping on the electronic structure of crystals, and physical properties of polymers. The simulation tools use density functional theory (DFT) and molecular dynamics (MD) and have been designed with non-expert users in mind. These modules and tools have been used, in conjunction with experiments, in several core undergraduate courses in Purdue's School of Materials Engineering and exemplify how simulations and experiments complement each other in an ICME approach.

8:40 AM
Towards an ICME Methodology- Current Activities in Europe: *Georg Schmitz*[1]; [1]Access E V
Scope of this presentation is to provide an overview about activities towards an ICME methodology currently going on in Europe. It will introduce the European Materials Modelling Council (EMMC) and provide an outline of its activities. One objective is a standardized nomenclature aiming to facilitate interoperability between software tools in the area of electronic, atomistic, mesoscopic and continuum descriptions of materials. A possible path of interoperability between scientists and engineers aiming at "engineering the material" with the FEM community focusing on "engineering with materials" is based on an HDF5 description of materials allowing both statistical and spatially resolved microstructure data being easily exchangeable. Respective simulation scenarios can be deployed as workflows on simulation platforms and on future materials modelling marketplaces.The research leading to these results has been performed within the EMMC-CSA and MarketPlace projects under grant agreements n° 723867 and n° 760173

9:00 AM

The Materials Commons: A Collaboration Platform and Information Repository for the Global Materials Community: *Brian Puchala*[1]; Glenn Tarcea[1]; Tracy Berman[1]; Steve DeWitt[1]; John Allison[1]; [1]University of Michigan

The Materials Commons is an information repository and collaboration platform developed by the PRedictive Integrated Structural Materials Science (PRISMS) Center at the University of Michigan. The Materials Commons provides a common place for researchers to store project files and data with provenance information, privately share them with collaborators, and then publish completed datasets for the entire community to use. This talk provides an overview of the Materials Commons with example use cases. We will highlight newly developed features including i) data ingest via spreadsheet uploads, ii) data ingest using Globus file transfer, iii) integrations with PRISMS Center software, and iv) integrations with the broader materials data infrastructure community. Finally, we will discuss future directions and opportunities for collaboration.

9:20 AM

Achieving Complete Interoperability in Materials Data: *Matthew Jacobsen*[1]; Charles Ward[1]; [1]US Air Force

Great strides have been made recently in the ICMSE community with the widespread adoption of flexible databases and best practice Application Programming Interfaces (APIs). Tremendous connectivity has been enabled between dozens of systems representing as many organizations. In spite of these achievements, a significant barrier to fully achieving "FAIR" principles – findable, accessible, interoperable, reusable – persists in the creation of data and schemas that are syntactically and semantically interoperable. Failures arise when multiple systems attempt to transfer data, stemming from a lack of common structure, description, or relation. In response to these challenges, the Air Force Research Laboratory (AFRL) has created a software platform called HyperThought™ that allows end users to create formal data structures and schemas for both concept and context definition. This presentation will show the benefits of FAIR-compliant, community-defined data structures by examining use cases in Additive Manufacturing, Machining, and Microscopy.

9:40 AM

Standardization of Materials Representation through Metamodeling Based Ontology: Sreedhar Reddy[1]; *B. Purushottham Gautham*[1]; Prasenjit Das[1]; Reghavendra Reddy Yeddula[1]; Sushant Vale[1]; Gerald Tennyson[1]; Rishabh Shukla[1]; Srimannarayana Pusuluri[1]; Akash Bhattacharjee[1]; [1]Tata Cunsultancy Services

Digital enablement of ICME would require standards for representing various entities of interest. Central to this is the representation of materials across all contexts of interest, i.e. an ontology. In this paper, we present a method for developing an ontology for representation of materials at various levels of abstraction. We start with a metamodel that provides foundational concepts necessary to describe materials, e.g., "a material has a composition", "composition comprises of elements and/or chemical compounds", etc. This metamodel is used to describe specific material class "subject models". For example, subject model of "steel" has specialized representation of composition through elemental weight percentages. Finally, an individual manifestation of steel with numerical attribute values is represented using the subject model as the semantic basis. The paper will describe details of this hierarchical modelling of materials ontology supported with examples on how this has been realized in a digital platform TCS PREMAP.

10:00 AM Break

10:30 AM Invited

MatCloud: A High-throughput Computational Infrastructure for Integrated Management of Materials Simulation, Data and Resources: *Xiaoyu Yang*[1]; [1]Computer Network Information Center of the Chinese Academy of Sciences

MatCloud is a Cloud-based computational infrastructure for the integrated management of materials simulation, data and computing resources. It is directly connected to a computing cluster and a materials simulation database, integrating the computing facilities, data, various scripts, and simulation code together to automatically manage the creation and running of simulation jobs, the subsequent extraction of core output information, the longer-term archival of materials properties data. One of important novelties of MatCloud is it provides a graphical user interface for end user to create a customised workflow for running materials simulations. Once simulation completes, the required materials properties have been acquired and preserved in the database. The more users use MatCloud, the more simulation data in MatCloud will be accumulated (for using licensed software such as VASP user must provide license). If users do not wish their data open to public, they can set their data not searchable by others.

10:50 AM Invited

Materials Ontologies for Knowledge Representation in ICME: *Gandham Phanikumar*[1]; [1]Indian Institute of Technology Madras

In an ICME implementation that integrates models, propagation of assumptions across the integration chain is important to ensure the validity of the approach. Asserting the readiness of a materials criterion as a digital / computable one will also bring more models into the ICME approach. The ecosystem to represent such knowledge has matured today: OWL 2.0 standard, editors for knowledge bases, reasoning engines, SPARQL for querying, SWRL to generate rule based assertions, OntoGraf for visualization of relationships and OWL-api to prepare assertions in a programmatical manner are now freely available. The expressivity provided by this ecosystem can capture fairly complex knowledge. Useful inferences with satisfactory depth of knowledge can be drawn and explained by reasoning engines. Ontologies also provide a platform to capture the knowledge of a domain expert in the form of assertions about the model assumptions, limitations of theories and validity of generalizations that can be carried forward as the model linkages are prepared during vertical integration. The following use cases will be presented: (a) An integration of crystallography knowledge with the data of materials project repository (b) Assertion of digital criteria for manufacturing defects relevant to additive manufacturing (c) Capturing computing process workflows.

11:10 AM

Workflow Manager for High-throughput DFT Cloud Calculations: Alejandro Strachan[1]; *Austin Zadoks*[1]; [1]Purdue University

Workflow managers for materials science applications are useful tools for high throughput studies, provenance tracking, and data sharing. Growing interest in combining data science and simulation to predict materials properties and discover new materials has driven the development of many advanced and powerful workflow managers. Despite their power, the heavyweight requirements of these workflow managers including external database servers make them impractical for instance-based cloud tools. We describe the design and implementation of a lightweight workflow manager created for cloud computing on nanoHUB.org. The tool provides support for density functional theory calculations through an API accessible in Jupyter notebooks and data storage in a local object-based database. Without installing any local codes or software, users have access in their browser to a programmable workflow manager, provided workflows and examples, and the computational resources of nanoHUB.org.

11:30 AM

Development of a Comprehensive Diffusion (Mobility) Database for Lightweight Mg Alloys: *Wei Zhong*[1]; Ji-Cheng Zhao[1]; [1]Ohio State University

Insufficient diffusion coefficient data of Mg alloys especially for some key alloying elements are hindering the computational design of high performance Mg alloys using the ICME (Integrated Computational Materials Engineering) approach. High-throughput diffusion multiples and novel liquid-solid diffusion couples are combined with a forward-simulation analysis to extract a large amount of diffusion coefficients of several essential alloying elements in Mg alloys, including Al, Zn, Sn, Ca, Mn, Li, Y, Gd and Ce. Together with the critically evaluated literature data, a comprehensive and reliable diffusion coefficient database for Mg-based systems is established. These experimental diffusion coefficient data together with thermodynamic databases as well as first-principles calculation results are used to establish a mobility database for CALPHAD modeling of processes and properties of Mg alloys; and thus will contribute to the accelerated development of next-generation Mg alloys.

11:50 AM

A Knowledge Engineering Framework for Knowledge Assisted Design in ICME: Raghavendra Yeddula[1]; Sushant Vale[1]; Sreedhar Reddy[1]; Chetan Malhotra[1]; *Gautham B. Purushottham*[1]; Yogesh Tambe[1]; [1]Tata Consultancy Services

Design is a knowledge-intensive activity and integrated design requires a designer to leverage knowledge cutting across several design domains. The designer needs access to right knowledge at right points in the design process for making right design decisions. To enable this, it is essential to understand the context in which a decision is being made so that right knowledge can be delivered. We give an overview of a knowledge engineering framework we have developed as part of our ICME platform, TCS PREMAP. We discuss how the framework helps in capturing knowledge cutting across different design domains catering to specific design needs, and how it helps in delivering knowledge in a context sensitive manner. We show how such context sensitive knowledge helps set up right workflows for a given design problem, and helps provide right guidance while executing them. We present this with case studies in material and product design.

ICME 2019 — Special Topic: Lightweight Innovations for Tomorrow (LIFT) Review

Tuesday AM
July 23, 2019

Room: White River I-J
Location: JW Marriott Indianapolis

Session Chairs: John Allison, University of Michigan; Tracy Berman, University of Michigan; Challan Park, University of Michigan

8:00 AM

Location-specific Microstructural Prediction of Forged AA2070 Parts: *Luke Borkowski*[1]; Alex Staroselsky[1]; [1]United Technologies Research Center

A new generation of Al-Li alloys offers weight savings while also providing other property benefits such as good strength and toughness combination. The forging of such alloys for aircraft engine parts leads to lower weight, improved performance, and longer life. Detailed analyses are needed in order to connect processing parameters to location-specific part microstructural characteristics and properties. Therefore, a physics-based, non-isothermal, visco-plastic crystal plasticity (CP) model has been developed to predict the microscale evolution that occurs in Al-Li during forging operations. The model considers the effects of rate-dependent plasticity, dynamic recovery, and dynamic recrystallization, all of which have been shown to influence the final microstructure in forged Al-Li parts. The calibrated CP model has been coupled with a commercial FEA software to perform forging simulations. Validation includes predicting the constitutive response of AA2070 under axial loading at multiple strain rates and temperatures and final location-specific texture of a forged part.

8:20 AM

ICME Approach to Predicting Texture Evolution of an Al-Li Alloy during Thermomechanical Processing: *Challan Park*[1]; Tracy Berman[1]; Veera Sundararaghavan[1]; John Allison[1]; [1]University of Michigan

An Integrated Computational Materials Engineering (ICME) approach was adopted to develop the LIFT multi-scale numerical framework that can accurately predict the evolution of local microstructure of metallic alloys during thermomechanical processes. The framework consists of a crystal plasticity (CP) user subroutine integrated into DEFORM software. The macroscopic forging simulation is handled by the DEFORM solver while the local texture evolution is calculated via the CP subroutine. The crystallographic texture is represented by the orientation distribution function while a rate-independent constitutive model is employed to maximize computational efficiency. To accurately update the ODF for high-strain conditions, Lagrangian ODF conservation and ODF remapping schemes are adopted. This LIFT numerical framework was validated with experimental characterization of the texture evolution during thermomechanical processing of a third generation aluminum-lithium alloy, AA2070. A Gleeble thermomechanical simulator and Electron Backscatter Diffraction (EBSD) were used to characterize the evolution of texture.

8:40 AM

LIFT TMP R4-6: ICME Approach to Linear Friction Welding of Ti-6Al-4V: *Austin Mann*[1]; Samuel Kuhr[2]; Kaiwen Zhang[2]; Michael Eff[3]; Wei Zhang[2]; Hamish Fraser[2]; [1]Boeing Research & Technology; [2]The Ohio State University; [3]Edison Welding Institute

The current state of the aerospace industry places an extraordinary demand on cost reduction of metallic materials. A potential solution is to enable linear friction welding (LFW) for production of net-shape titanium pre-forms, leading to cost reductions in raw materials and processing. Accelerated implementation of LFW (particularly for Ti-6Al-4V) is limited by extensive qualification and certification, incomplete databases as inputs to predictive models, geometric effects on process robustness, and an understanding of microstructural evolution as a function of process parameters. It is imperative that an Integrated Computational Materials Engineering (ICME) tool be developed to model the LFW process. In this effort, an ICME approach was utilized to build a manufacturing simulation package for LFW of Ti-6Al-4V. This includes detailed process characterization via in-situ measurement techniques, generation of high fidelity material data at representative conditions, and component validation of modeling techniques on one of the largest LFW machines in North America.

9:00 AM

In-situ Measurement and Numerical Simulation of Linear Friction Welding of Titanium Alloy: *Kaiwen Zhang*[1]; Wei Zhang[1]; Samuel Kuhr[1]; Hamish Fraser[1]; Michael Eff[2]; Austin Mann[3]; [1]Ohio State University; [2]EWI; [3]Boeing Research & Technology

Linear friction welding (LFW) is a solid-state joining process that is currently used in the aerospace industry for joining titanium alloy structures (e.g., blisks), and increasing being utilized for fabricating net-shape titanium pre-forms. The process is highly transient involving rapid heating and cooling, severe plastic deformation and dynamic recrystallization. A finite element model for LFW was developed to improve the quantitative understanding of material thermal and deformation histories. Specially-designed LFW experiments were performed with Ti-6Al-4V, painted with speckle patterns to map the surface deformation in-situ by digital image correlation (DIC). Multiple thermocouples through drilled holes were used for tracking temperature profiles near the faying interface. Gleeble™ based thermo-mechanical simulations were performed to generate high temperature stress-strain data at relevant strain rates. 2D/3D LFW models were developed base on DEFORM, a commercial finite element code. Calculated temperature and deformation results were correlated to the gradient of microstructure across the joint.

9:20 AM

Linear Friction Welding of Ti Components: Investigation of Residual Stress and Fatigue Performance: Ritwik Bandyopadhyay[1]; *Michael Sangid*[1]; [1]Purdue University

Linear friction welding, of similar or dissimilar Ti alloys, offers a promising technology for producing large, net shaped components with assured or tailored properties. The residual stresses of Ti64-Ti64 and Ti64-Ti5553 welds are quantified via energy dispersive x-ray diffraction for the as-welded and post-weld heat treatment conditions, and the associated microstructures are analyzed by backscatter electron imaging. For these materials, fatigue failure is prone to occur in the Ti64 base material, which experiences anomalous fatigue behavior at high R ratios. To investigate this phenomenon, strain accumulation and crack initiation are investigated in various samples with and without microtextured regions via high-resolution digital image correlation and complemented with crystal plasticity modeling. In this work, the anomalous mean stress behavior experienced by Ti64 at high R ratios is explained by high creep sensitivity, activation of the pyramidal slip systems, and degree of micro-plasticity resulting in increased fatigue damage at high R ratios.

9:40 AM

Development of Computational Tool for Predicting the High Temperature Gas Pressure Forming of Titanium Beta 21S.: *Anthony Clinton*[1]; Chal Park[2]; Martin Philo[1]; Fernando Alamos[3]; David Go[3]; Steven Schmid[3]; [1]GKN Aerospace; [2]University of Michigan; [3]University of Notre Dame

The creep form process enables the fabrication of complex contoured components from initially unstrained material, with significantly reduced thinning compared to plastic deformation processes. Computational modeling using the finite element method (FEM) is an essential part of the process development cycle and is necessary to minimize development time and tooling costs. Accurate material models are needed for high confidence in simulation results. Creep models that come with most commercial FEM software are simple and do not sufficiently recreate the creep form process. To improve design and manufacturability, in this work, a sophisticated FEM-based numerical framework is developed that can accurately predict material behavior during the entire creep process. The high temperature creep behavior is modeled by the Wilshire Extrapolation Technique, while the friction behavior is modeled by an advanced function of various state variables. The proposed framework was calibrated based on the material characterization and friction testing of Titanium β21S.

10:00 AM Break

10:30 AM

Robust Distortion Control and ICME Implementation to Support Ship Production Processes: *T.D. Huang*[1]; Steven Scholler[1]; Yu-Ping Yang[1]; Randy Johnson[1]; Charles Fisher[2]; Wei Zhang[3]; San Gooroochurn[4]; Theodor Freiheit[5]; [1]Huntington Ingalls Industries; [2]NSWC-Carderock Division; [3]The Ohio State University; [4]ESI - North America; [5]The University of Michigan

The shipbuilding process has historically experienced the introduction of steel plate distortion in the earliest stages of construction and from downstream processes. Distortion starts when thin steel plates are butt-welded together to create larger panels, and when structural stiffeners are welded to them. These distortions can result in increased sub-assembly fitting-time, welding, labor costs, and schedule impact to ship production. The gaps between stiffened panels must be reduced to facilitate optimum coplanar plate proximity for welding. Insufficiently mitigated distortion in the final stage of production could impact the ship's maneuverability efficiency and mission capability. Funded by the Navy ONR through the Lightweight Innovation for Tomorrow (LIFT) consortium, this project aims to address these production issues through the development of novel, multi-scale, Integrated Computational Materials Engineering (ICME) techniques that can be readily applied in shipyard fabrication processes in order to improve product quality and reduce overall lightweight steel manufacturing costs.

10:50 AM

Development of ICME Methods to Improve High Pressure Die Casting (HPDC) Technologies for Thin-wall Aluminum Components: *Tracy Berman*[1]; Diran Apelian[2]; Alan Luo[3]; Jiten Shah[4]; John Allison[1]; [1]University of Michigan; [2]Worcester Polytechnic Institute; [3]The Ohio State University; [4]Product Development & Analysis (PDA)

This project focused on the development of High Pressure Die Casting (HPDC) technologies for aluminum alloys that are required for producing high quality thin-wall aluminum die cast components. Existing computational tools, including CALPHAD and HPDC casting simulations, and current best practices were used to inform the alloy selection, die design, and casting processes. The manufactured HPDC Al-Si-Cu-Mg alloy (LIFT380) components were distributed for microstructural characterization, heat treatment process development, and mechanical testing. Experimentally calibrated computational tools, were used to predict the grain size, solute concentration, and precipitate structure in heat treated LIFT 380 components. These outputs were then incorporated into a physics-based strengthening model that was demonstrated to accurately calculate yield strength. The results from this work are being incorporated into ICME tools which predict location-specific properties and can be used to accelerate the design and optimization of high pressure die cast components and processes.

11:10 AM

Application of ICME towards Thin Wall Casting Technology Development at LIFT: *Jiten Shah*[1]; [1]PDA LLC

Casting process modeling of filling and solidification has been in use by OEMs and casting producers for over two decades and the ICME models have matured over the recent past. For the design and development of thin wall casting configurations, it is critical to asses the impact of higher cooling rates due to thinner walls on the micro-structure and mechanical properties. The presentation will share the ICME work conducted from projects funded by LIFT (Lightweight Innovations for Tomorrow, a Manufacturing USA public-private partnership) towards the development of thin wall super vacuum high pressure die casting aluminum and sand cast iron casting technologies. The key aspects of ICME model calibration, verification and validations will be presented with case studies.

11:30 AM

Coupling Experiments and Simulations to Predict Microstructure and Yield Strength in Precipitation Hardened Aluminum Alloys: *Qianying Shi*[1]; Tracy Berman[1]; Jacob Garves[1]; John Allison[1]; [1]University of Michigan

Three aluminum alloys, an Al-Cu-based high pressure die casting alloy (LIFT380), an Al-Mg-Zn-based rolled alloy (AA7075), and an Al-Cu-Li-based forged alloy (AA2070) were used in this study to develop the LIFT-ICME methodology for the modelling of microstructural evolution and yield strength for age hardened alloys. Systematical experimental measurements and simulations were performed to build the linkage between manufacturing history, microstructure and yield strength for each specific alloy. Using commercial CALPHAD software, microstructural evolution during solidification and heat treatment was simulated by calibrated thermodynamic and kinetic models. These microstructural evolution simulations have been used in conjunction with physics-based linear superposition strengthening models to predict the yield strength for investigated aluminum alloys, which all are significantly strengthened by precipitation. This integrated approach can be used to optimize alloy compositions, manufacturing processes and engineering products.

11:50 AM Invited

LIFT ICME: A Strategic Initiative for Accelerating Manufacturing Innovation of Metallic Materials: *John Allison*[1]; Chal Park[1]; [1]University of Michigan

Integrated Computational Materials Engineering (ICME) is a transformative discipline that has the potential to revolutionize the way new products, materials and manufacturing processes are developed and optimized. The LIFT (Lightweight Innovations for Tomorrow) consortium is a US manufacturing innovation institute with over 100 member companies, universities and other organizations and is focused on developing and implementing advanced manufacturing solutions for the metals industry. ICME is considered a core and critical enabling technology for LIFT. To address the challenges this presents and provide industry-ready ICME capabilities to LIFT members, a broad-based LIFT ICME program has been defined and initiated. The key elements of the LIFT ICME strategic plan are development of advanced tools & methods, developing solutions for ICME Foundational Engineering Problems (FEPs), providing industry-ready software and materials information infrastructure and training/retraining the required ICME workforce. This talk will provide an overview of LIFT ICME successes and plans for the future.

ICME 2019 — Application: Future Developments

Tuesday PM
July 23, 2019

Room: White River F
Location: JW Marriott Indianapolis

Session Chair: Charles Fisher, Naval Surface Warfare Center - Carderock

2:00 PM Plenary

An ICME Approach for Additive Manufacturing: TK Ales[1]; A Baker[2]; HL Fraser[3]; DG Harlow[4]; Y Wang[3]; *Peter Collins*[1]; [1]Iowa State University; [2]Boeing; [3]The Ohio State University; [4]Lehigh University

Increasingly, additive manufacturing is being adopted to produce near net-shape metallic parts for various applications. However, given the relative lack of design allowables, and the expense of developing the appropriate datasets, a new strategy of qualification is required. One such strategy is known as "informed qualification", where simulation tools and models, along with limited data, can be used to ascertain relatively quickly whether a manufacturing process, characterized by a process window, will result in acceptable quality of components. This type of rapid, informed qualification framework is built upon an ICME philosophy, where the objective is to rapidly obtain sufficient data to render an informed, engineering solution. This talk will present such a framework, while simultaneously addressing the complicated physics associated with the additive manufacturing process and the resulting deposited materials composition, microstructure, properties, and performance. In this approach, we link macroscopic thermal models to a Langmuir approach to predict composition, both of which are linked to microstructure models, all of which feed into property predictions. Finally, a statistically based strategy that permits the resulting, final model to be calibrated with limited data to accurately predict performance, as measured by cumulative probability distribution functions of the properties. While there have been significant breakthroughs in this work, and while our predictions of design allowables are within 1% of experimental observations, we have also uncovered areas which require far more work. These emerging areas will also be discussed.

2:40 PM Plenary
Using 3D Characterization to Establish Structure Processing Relationships in Additive Manufacturing: *David Rowenhorst*[1]; [1]Naval Research Laboratory
The additive manufacturing process yields highly complex microstructures when compared to the traditional processing methods. Furthermore, because the parameters and heat input are location dependent with a build, 3D characterization methods are necessary to capture the influence of these localized processing parameters on the microstructure and thus the resultant properties. Here we will present the results of using multiple 3D techniques including high-resolution x-ray tomography to examine pores within the material non-destructively, as well as 3D serial sectioning which reveals the the true 3D grain shapes and crystallographic textures within laser bed fusion 316L stainless steel. We will not only show that the morphologies in these structures are directly related to the local processing, but that these structures are dramatically different than what is found in traditional 316L microstructures.

3:20 PM Break

3:40 PM Plenary
Integrated Computational Materials Engineering (ICME): Past, Present, and Future: *Mark Horstemeyer*[1]; [1]Liberty University
Integrated Computational Materials Engineering (ICME) as reflected by hierarchical multiscale modeling along with modeling the Process-Structure-Property-Performance (PSPP) sequence will be discussed with several applications demonstrating the methodologies. This modeling methodologies will be shown to address a broad range of engineering problems. To predict the performance of a structural component, an analyst needs to consider the microstructure-property relationship to capture material history effects in the constitutive relations when performing the simulations. An effective method to capture the microstructure-property relationship is by use of internal state variable evolution equations, which reflect lower spatial size scale microstructural rearrangements so that history effects can be modeled. Also, educational issues will be addressed with respect to an ICME course that has been taught with residence and online students at Mississippi State University. Finally, the past, present, and future will be discussed in the aforementioned context.

4:20 PM Plenary
To Be Announced: *Michele Manuel*[1]; [1]University of Florida

ICME 2019 — Industrial Usage of ICME Techniques

Wednesday AM
July 24, 2019

Room: White River F
Location: JW Marriott Indianapolis

Session Chair: Charles Fisher, Naval Surface Warfare Center - Carderock

8:00 AM Plenary
The Opportunities and Challenges in Embedding Materials Science in Virtual Design and Manufacturing: *Mary Lee Gambone*[1]; [1]Rolls-Royce Corporation
This is an exciting time to be a materials engineer! Revolutionary capabilities such as data informatics, virtual reality, and artificial intelligence are really starting to transform what we can do to understand materials and predict their behavior in applications. And this is not too soon – the need for new materials and the desire to adopt new materials production methods are challenging our traditional approaches that are dominated by extensive experiment and characterization. In this presentation I will discuss some examples to illustrate the art of the possible for behavior prediction and uncertainty quantification using computational materials engineering methods as well as some the barriers that continue to slow the progress of development and application.

8:40 AM Plenary
Titanium Alloy and Process Design: Gaining Insights through Multi-scale Computation: *Rui Yang*[1]; [1]Institute of Metal Research
Titanium alloys possess a rich variety of phase transformations and multi-scale microstructures, and computing and simulation at different scales can play significant roles in composition design, microstructure optimisation and property improvement. This talk will review work conducted in the past few years using such an experiment plus computation approach, taking examples from near-alpha titanium alloys and titanium aluminides for aero engine applications and from beta-type titanium alloys for biomedical and marine use. Such an integrated approach accelerates the optmisation process and in many cases sheds new light on unresolved problems. The topics to be covered include alloying effects on the alpha phase and their relations to creep resistance and cold dwell fatigue propensity, alloying effects, phase stability and deformation mechanisms of high strength titanium aluminides, and metastable phases and stress induced transformations in beta-type titanium alloys.

9:20 AM Plenary
Development of Metallurgical through Process Models for the Development of New Low Carbon Strip Steel Grades: Kees Bos[1]; *Jesús Galán-López*[2]; [1]Tata Steel Europe; [2]TU Delft
The mechanical properties of modern low carbon strip steel grades are increasingly sensitive to steel-mill process conditions. Because real full-scale process conditions can be difficult to reproduce in a laboratory, physically based metallurgical through process models that can be calibrated with laboratory data, but which can also describe the microstructure evolution under actual mill conditions, are increasingly valuable for the development and optimization of new steel grades. In this work recent additions to the physical Cellular Automata Sharp Interface Phase Transformation (CASIPT) model in the areas of diffusion, recrystallization and phase transformation are presented. Furthermore, examples of how the CASIPT model can be combined with empirical metallurgical models are provided. This in turn illustrates how the CASIPT model can be incorporated into a complete through process model chain, from the hot strip mill reheating furnace up to the continuous annealing line, and thus used for new grade development.

10:00 AM Break

ICME 2019 — Industrial Integration and Success Stories I

Wednesday AM
July 24, 2019

Room: White River F
Location: JW Marriott Indianapolis

Session Chair: Vasisht Venkatesh, Pratt & Whitney

10:30 AM Invited
Business Transition Considerations for Integrated Computational Materials Engineering: *Satyam Sahay*[1]; Mohamad El-Zein[2]; Goutam Mohapatra[1]; [1]John Deere Asia Technology Innovation Center; [2]John Deere Moline Technology Innovation Center
A framework of ICME was developed with simultaneous optimization of design, materials and manufacturing. This framework was leveraged for several tractor casting components, with accelerated development cycle and robust product. This article will discuss about technology development cycle in industry from prospecting to research, development and business transition of a new competency. Important aspects of multifunctional nature of new competencies necessitating a new approach to teaming and workflow will be discussed. Furthermore, the limitation of prevalent ICME frameworks in managing dynamic asymmetric commodity price fluctuations will be highlighted with specific examples. A modified ICME framework will be presented, where commodity price fluctuation is explicitly included to provide material optionality at the product development stage. This framework will enable supply chain in an OEM to make medium and long term strategic decision for prioritizing grades, which has low impact on commodity price volatility.

10:50 AM

An ICME Modeling Application in Aircraft Tie-down Design Improvement for Ship Production: T.D. Huang[1]; Yu-Ping Yang[1]; *Steven Scholler*[1]; Randy Johnson[1]; [1]Huntington Ingalls Industries

Aircraft tie-downs have been widely used to secure aircrafts to a ship's deck. Tie-downs are heat treated by a quenching, tempering, and carburizing process to achieve the strength and surface hardness. The high surface hardness could result in low ductility and lead to cracking with the weld-induced residual stress and compounded when external loads are applied. This is a major concern because the tie-downs are subject to cyclic, dynamic loading which could induce cracking during services under sea-state loading conditions. ICME models including thermo-mechanical models were used to optimize the welding sequence and geometry designs to reduce weld residual stress. It was found that the corners of tie-downs have the highest weld residual stress and increasing the corner radius can then significantly reduce the possibility of cracking or crack initiation points. Experiments were conducted to validate the modeling predictions on the current baseline and the proposed designs.

11:10 AM

A Digital Twin for the Design Space of Welded Structures: *John Goldak*[1]; [1]Goldak Technologies Inc.

This paper describes VrWeld, a multi-physics multi-scale digital twin to design optimal experiments to assess the product performance and manufacturing cost. The quasi-static arc weld pool model that conserves mass, energy and momentum and includes gravity and surface tension supports the analysis of multi-position, multi-pass welds as a function of the weld joint design and weld procedure. The correlation of multi-sensor experimental data with virtual data predicted by the digital twin for several welding experiments is discussed. Several industrial design problems are discussed including designs for the repair of a nuclear reactor, machinery, natural gas pipelines and wide flange beam structures. The capability to do global optimization in a design space is discussed. It is expected that next generation digital twins will be coupled with sensor networks and robots to provide model-based real-time control of the welding process.

11:30 AM

Modeling Long-term Creep Behavior of Power Plant Steels: *Abhinav Saboo*[1]; Changning Niu[1]; Jiadong Gong[1]; Qiaofu Zhang[1]; [1]QuesTek Innovations LLC

The efficiency of steam power plants can be increased by operating at a higher steam pressure and temperature. Realizing such improvement requires cost-competitive materials with desired long-term creep performance. QuesTek Innovations LLC, a leader in the field of computational materials design, developed a robust creep modeling toolkit that expands its computational Materials by Design® technology, in order to predict the long term creep behaviors of P91 steels in fossil energy systems. The developed model is built on science-based mechanisms (not empirical approach) with improved predictive capability over traditional empirical approaches for reliable lifetime assessments and maintenance of power plant components.

11:50 AM

Cloud-based Materials and Products Realization – Fostering ICME via Industry 4.0: *Anand Balu Nellippallil*[1]; Zhenjun Ming[2]; Janet K. Allen[2]; Farrokh Mistree[2]; [1]Center for Advanced Vehicular Systems, Mississippi State University; [2]Systems Realization Laboratory, The University of Oklahoma

Fostering ICME in the globalized 21st century demands a need to facilitate a network of participants (material scientists, systems designers, customers) to share material/product/manufacturing process/market data, information, knowledge, and resources instantly and collaborate so as to facilitate a cost-effective co-creation of value supporting open innovation. Industry 4.0, a transformative industrial revolution with its new product development paradigms like cloud-based design and cloud-based manufacturing supports this need.In this paper, we present the architecture and functionalities of a cloud-based computational platform to facilitate mass collaboration and open innovation thereby supporting material and product realization needs to institutionalize ICME in industry. We illustrate the efficacy of the proposed cloud-based platform using a hot rolling example problem to produce a steel rod. Using this example, we demonstrate the utility of the cloud-based platform in seamless, yet controllable, information, knowledge, and resource sharing thereby supporting the integrated design of materials, products, and manufacturing processes.

ICME 2019 — Linkage: Process-Microstructure I

Wednesday AM
July 24, 2019

Room: White River I-J
Location: JW Marriott Indianapolis

Session Chair: To Be Announced

10:30 AM

ICME-based Approach to Design Quench and Partition (Q&P) Steels: *Amit Behera*[1]; Greg Olson[2]; [1]QuesTek Innovations LLC; [2]Northwestern University

Q&P alloys belong to the 3rd generation of AHSS that are known to showcase excellent combination of high strength along with good ductility. The key microstructural features affecting ductility in these alloys is the austenite stability which is mainly controlled by the austenite carbon content and its morphology after Q&P processing. The current work discusses predictive design of composition and processing of these martensite/austenite TRIP steels utilizing the theory of coupled diffusional/displacive transformation and highly accurate experimental measurements including high energy x-ray diffraction, 3D atom-probe tomography. Mechanistic models to predict the role of alloy composition and process parameters on the final structure and properties have been developed and experimentally validated. The cross-linkage between processing-structure-properties for design of new alloys will be discussed.

10:50 AM

Bayesian Framework for Inverse Inference in Manufacturing Process Chains: *Avadhut Sardeshmukh*[1]; Sreedhar Reddy[1]; BP Gautham[1]; [1]TRDDC, TCS Research, Tata Consultancy Services, Pune, India

Process-property relations are central to ICME. Engineers are often interested in using these relations to make decisions on process configurations to achieve desired properties. This is known as the inverse problem and it is typically solved using forward models (physics based or data based) in an optimisation loop, which can sometimes be expensive and error prone, especially when used on process chains with multiple unit steps. In this paper we propose a Bayesian networks based approach for modelling process-property relations that can be used for inverse inference directly. We also discuss how unit process models can be composed to do inverse inference on the process chain as a whole. We demonstrate this on a wire-drawing process where a wire is drawn in multiple passes to achieve desired properties. We learn a Bayesian network for a unit pass and compose it multiple times to infer process parameters of all passes together.

11:10 AM

A Crystal Plasticity Model for the Prediction Quench Cracking of Carbon Steels: *Prashant Jadhav*[1]; Hector Basoalto[1]; Christopher Watson[2]; [1]University of Birmingham; [2]Rolss-Royce plc, Derby, UK

Quenching of carbon steels is an established process for the improvement of mechanical properties; however these materials are susceptible to quench cracking and the conditions leading to failure are not well understood. This study presents a physics-based, multi-scale materials modelling framework for the prediction of quench cracking conditions. The rapid cooling rates associated with the quenching process induce high thermal and transformational strains which provide the driving force for the nucleation, growth and coalescence voids that eventually form cracks. This work focuses on the prediction of the trans-granular void initiation conditions associated with decohesion events at austenite/martensite interfaces. A phenomenological plasticity model has been developed to identify conditions for crack initiation based on the violation of compatibility conditions on the deformation fields between phases. Based on these conditions, definition of damage variables at the meso and macro-scale are developed.

11:30 AM

An Integrated Approach to Simulating and Characterizing Gamma Prime Precipitation in Nickel Superalloys: *Nicholas Krutz*[1]; Chen Shen[2]; Jiashi Miao[1]; Justin Bennett[3]; Wei Zhang[1]; Michael Mills[1]; [1]Ohio State University; [2]GE Global Research; [3]GE Aviation

A multi-scale heat treatment simulation of a gamma-prime strengthened nickel-base superalloy is presented and validated using thermal analysis and 3D microstructure reconstruction. A mean-field model of the gamma prime precipitation is used to predict the nucleation and growth for two nickel superalloys under fast and slow continuous cooling of small-scale lab specimen. The predicted volumes of the precipitates are compared to 3D reconstructions obtained using Focused Ion Beam serial sectioning. The multiple nucleation burst events known to this alloy type are characterized by in-situ cooling experiments and compared

to predictions. Spatial effects of the gamma prime evolution are obtained by applying the model to the element integration points of a FEM-based heat transfer model to approximate rate-dependent latent heat effects. The heat released during the evolution is shown to have a cascading effect on the overall heat transfer observed, the implications of which are demonstrated using embedded thermo-couple experiments.

11:50 AM

Crystal Plasticity Simulation of Fatigue Behavior in Rolled Magnesium Alloy: *Fabien Briffod*[1]; Takayuki Shiraiwa[1]; Manabu Enoki[1]; [1]The University of Tokyo

The present study focuses on the experimental investigation and modeling of the mechanical behavior of rolled magnesium alloy under fatigue conditions. A phenomenological crystal plasticity model accounting for twinning, detwinning and slip in the twinned region is considered and calibrated against monotonic and cyclic experimental data. Periodic two-dimensional polycrystalline aggregates are generated based on statistical data obtained from electron backscattering diffraction measurements and a proposed anisotropic tessellation. The microstructures are loaded under cyclic conditions at different stress amplitudes and mesoscopic non-local fatigue criteria for slip and twin-induced crack initiation are estimated. The sensitivities of the criteria in terms of mean behavior and relative dispersion against the stress amplitudes are compared with the results of load-controlled fatigue experiment. The limitations and predictive capabilities of the proposed approach are finally discussed.

ICME 2019 — Linkage: Structure-Properties I

Wednesday AM
July 24, 2019

Room: White River G-H
Location: JW Marriott Indianapolis

Session Chair: Qiang Feng, University of Science and Technology Beijing

10:30 AM

Crystal-plastic Modeling in the OOF Finite-element Solver: *Andrew Reid*[1]; [1]National Institute of Standards and Technology

The Object-Oriented Finite Element code (OOF) developed at NIST is a long-standing project to deliver high-quality computational modeling for materials science users. Recently, the development team has completed the addition of a family of crystal-plastic constitiuve rules, rounding out the solid-mechanics capabilities of the tool, and lowering the barrier for access to this important modeling capability. This effort was undertaken in collaboration with domain experts from the computational mechanics community. Being history-dependent, this expands the OOF project beyond its initial scope of what were essentially divergence equations. Incorporating the insights and algorithms of the computational mechanics experts into this general-purpose tool posed several challenges to the OOF team, but the result is a tool which can generate microstructural meshes from images, and allow users to plug in various crystal-plastic constitutive rules to their structure-property explorations.

10:50 AM

Multiscale Crystal Plasticity Simulation Based on Fatigue Indicator Parameters on Ultrafine-grained Metals: *Yoshiteru Aoyagi*[1]; David McDowell[2]; [1]Tohoku University/Georgia Institute of Technology; [2]Georgie Institute of Technology

Ultrafine-grained metals whose grain size is less than 1 micron have attracted interest as high-strength materials. In ultrafine-grained metals produced by severe plastic deformation such as accumulative roll bonding, the strong rolling texture induced by severe plastic deformation remarkably influences the anisotropy of mechanical properties. A computational model predicting the mechanical properties of ultrafine-grained metals is desired in the field of materials science and engineering. In this study, using results obtained by an electron backscatter diffraction method, information on crystal orientation is introduced into a computational model for crystal plasticity simulation considering the effects of grain boundaries and dislocation sources. Finite-element simulations for an aluminum plate under cyclic loading are performed to investigate a fatigue strength based on fatigue indicator parameters.

11:10 AM

Homogenization of 3D Metallic and Polymeric Microstructures in a ICME Context: *Gottfried Laschet*[1]; Mustapha Abouridouane[2]; Simon Koch[2]; Hamed Nokhostin[2]; [1]ACCESS e.V.; [2]RWTH Aachen University

A multiscale approach is applied here to predict effective properties of components, whose production is simulated on a ICME platform. At first, the austenite to ferrite phase transformation during cooling of a steel disc is presented. Effective thermo-elastic properties and a simulated dilatometer curve are derived. Then, the effect of the ferrite pearlite microstructure of a steel gear after annealing and before machining is analysed. Effective flow curves of the pearlite lamella, the ferrite matrix and of gear microstructures are derived. These curves are fitted by different ohnson-Cook hardening variants. To evaluate the machinability of the alloys, cutting simulations are performed and compared with cutting experiments. Finally, the multiscale simulation of an injection molding of a polypropylene plate is presented. After mold filling analysis, the spherulite microstructure evolution is predicted by a cellular automaton. A two-level homogenization is then used to predict local property variations over the plate thickness.

11:30 AM

Developing a Data-driven Model to Predict Microstructure-sensitive Spring Stiffness: *Aditya Venkatraman*[1]; David Montes de Oca Zapiain[1]; Hojun Lim[2]; Surya Kalidindi[1]; [1]Georgia Institute of Technology; [2]Sandia National Laboratories

Elastic constants of springs are dependent on many material and geometric parameters. A rigorous quantification of the spring constants' values would be computationally very expensive. Therefore, a more efficient method is required to accurately predict the spring constants. This study is aimed at developing a data-driven model that considers elastic constants and crystallographic texture in order to build a reduced-order model for the spring constant. A large number of CP-FEM simulations are conducted to develop a database of spring constants. A Gaussian Process Regression model is trained using the elastic constants and the Fourier Coefficients of the texture as input parameters and the spring constant as the output parameter. The model is shown to predict the spring constants very well, and enormous reduction in computing time is achieved compared to CP-FE simulations. Furthermore, this work provides a novel approach to understand microstructure-mechanical property relationship using data driven methods.

11:50 AM

Identifying Microscale Plastic Processes towards Optimized Mechanical Properties of Structural Materials via ICME: *Hao Wang*[1]; Gang Zhou[1]; William Wang[2]; Yanxia Liu[3]; Chunguang Bai[1]; Qing-Miao Hu[1]; Dongsheng Xu[1]; Jinshan Li[2]; Rui Yang[1]; [1]Institute of Metal Research; [2]Northwestern Polytechnical University; [3]Liaoning University

Employing state-of-the-art simulation techniques, we look into several important plastic processes, still undetermined due to the lack of understanding on the microscale deformation mechanisms of structural materials. The results indicate that, 1) There is no well-defined critical annihilation distance for dislocation dipoles in metals and alloys. Narrow dipoles are either transformable into clusters or stable over the experimental timescale. 2) Alloying elements vary both the stacking fault energy and the c/a ratio of hexagonal metals, thus affecting slip preference. 3) There exists a new twinning mode in γ-TiAl under the combination of anti-twinning shear and hydrostatic tension with relatively large strain and may contribute to ductility. 4) There is a critical lamella thickness ratio, below/above which the interface between γ-TiAl and a2-Ti3Al is coherent/semi-coherent, affecting the fatigue and fracture.The above microstructure parameters can then be incorporated into meso- and macro-scale models to evaluate the mechanical performance of structural materials.

ICME 2019 — Industrial Integration and Success Stories II

Wednesday PM
July 24, 2019

Room: White River F
Location: JW Marriott Indianapolis

Session Chair: Vasisht Venkatesh, Pratt & Whitney

2:00 PM Invited
Integrated Optimization of Liquid Metal Processing Operation and Upstream Operations: Abhishek Arya[1]; *Amarendra Singh*[1]; [1]Indian Institute of Technology Kanpur
Final liquid metal processing operation, prior to casting, often requires refining and alloying to meet the quality and composition specifications of the end product. In integrated process optimization, we often consider upstream processes of the metal production cycle. However, processes involved in production of refining agents and alloy productions are often ignored. In the present work, the importance of inclusion of such processes in optimization of liquid metal quality is highlighted through an example from steelmaking operation. In the present work, secondary steel making operation is linked not only with the upstream primary steelmaking operations but also with operations involved in formation and sizing of additives such as ferroalloys. Benefits of such integrated approach are highlighted in the context of integrated computational materials engineering and some key benefits in terms of energy and quality optimizations are presented.

2:20 PM
Modelling of Deformation Textures during Cold Rolling of SAF2906 Duplex Stainless Steel: Darshan Chalapathy[1]; *Sivaprasad Palla*[2]; Anand Kanjarla[1]; [1]IIT Madras; [2]Sandvik Materials Technology
It is of fundamental importance to study deformation in multi-phase materials with clear understanding like stress and strain partitioning among the phases, effect of orientation relationships etc. This study aims at modelling the deformation texture evolution in duplex stainless steels using rate independent crystal plasticity models with linear optimisation simplex method as solver. Grain interaction based LAMEL type models have been extended to a two-phase material with both slip and twinning as deformation mechanisms. Pre-dominant twin reorientation scheme is used to incorporate deformation twinning in austenite. The rate of texture development in austenite and ferrite is different and is related to initial textures and slip systems active in each phase. Deformation twinning in austenite is observed to play a significant role in texture development at higher strains. The effect of austenite on deformation of ferrite is substantial while the vice-versa is negligible and is also observed experimentally.

2:40 PM
ICME Assessment of Cladding Repair Processes: Daniele Bassan[1]; Ralf Reiche[2]; Olaf Rehme[2]; Josh Barras[3]; Joerg Willems[4]; *Mustafa Megahed*[4]; [1]CRF; [2]Siemens; [3]TWI; [4]ESI Group
Thermodynamic modelling is utilized to obtain temperature dependent alloy properties. Laser powder direct energy deposition process is modelled in detail to obtain bead characteristics including bead width, height and thermal history. Several beads are analyzed to ensure adequacy of the bead overlaps and achievement of dense deposits. Microscopic information is homogenized and transferred to workpiece analysis tools to predict as-built distortion and residual stress distribution. Workpiece specific fixtures are accounted for accordingly. The ICME platform is applied to two different industrial applications: Repair of a steam turbine blade and repair of an automotive tooling block.

3:00 PM
Modeling the Fatigue Performance of a Cast Polycrystalline Nickel Superalloy Using a Crystal Plasticity Approach: *Mark Veliz*[1]; Anssi Laukkanen[2]; Tomi Suhonen[2]; Matti Lindroos[2]; Tom Andersson[2]; [1]Caterpillar; [2]VTT Technical Research Centre of Finland
The performance of cast polycrystalline nickel-based superalloys has not been significantly studied in recent years due to the proliferation of single crystal alloys. However, it has been found that there are still advancements to be made in conventionally cast polycrystalline materials, particularly from a fatigue performance standpoint. Microstructures were characterized via SEM, EBSD, and micro-CT. and models were built using a crystal plasticity approach for an alloy with approximately 65% gamma prime phase fraction. Clean microstructures were compared with those incorporating defects such as free surfaces, grain boundaries, grain boundary carbides, and pores. It was found that while the intragranular gamma/gamma prime microstructure has a strong influence on fatigue performance, other microstructural constituents can be life-limiting. Detailed case studies are presented including real and synthetic defects. A good correlation with specimen failure data was demonstrated with the calibrated model.

3:20 PM Break

3:40 PM
Integrated Framework to Enable Engineering Realization of ICME for Iron Castings: *Ujjal Tewary*[1]; Shyamprasad Karagadde[2]; Alankar Alankar[2]; Goutam Mohapatra[1]; Satyam Sahay[1]; Indradev Samajdar[2]; [1]John Deere India Pvt. Ltd.; [2]Indian Institute of Technology Bombay
Cast iron continues to be a commercially important material for automobile industries. Graphite precipitates during the solidification process of the melt; its morphology, size, and distribution have significant impact on the mechanical properties. In this work, a microstructural model was developed to predict the size and number density of graphite during the casting process. This finite element framework is based on energy balance at the macro-scale; whereas at the micro-scale phase transformation kinetics is developed to predict the formation of graphite as a function of cooling rate. The validated prediction was coupled with a crystal plasticity finite element model to analyze the effect of morphology of graphite on interaction with the matrix. Local stress-strain map, texture evolution, and macroscopic stress-strain response because of various morphology of graphite are analyzed. The implication of this multiscale materials approach on the product development cycle, including design and manufacturing processes will be discussed.

4:00 PM
ICME Development of Carbon Fiber Composites for Lightweight Vehicles: *Xuming Su*[1]; David Wagner[1]; Jian Cao[2]; Mansour Mirdamadi[3]; Tim Foecke[4]; [1]Ford Motor Company; [2]Northwestern University; [3]Dow Chemical; [4]University of Maryland
"ICME Development of Carbon Fiber Composites for Lightweight Vehicles" was a DOE co-funded project, with a research team including Ford, Northwestern University, Dow Chemical, University of Maryland, LSTC, Autodesk, HBM and ESTECO.Mechanical properties of a composite depend not only on resin and fiber properties, but also layout of the fibers and the bonding between matrix and fibers. The numerical tools developed and integrated into ICME framework included those for preforming and compression molding simulation, multiscale models for continuous and chopped fiber composites which link material micro and meso structures to macro mechanical properties, crash analysis and testing and modeling methods of fatigue analysis. The ICME tools have been used for a simultaneous optimization of component design and manufacturing of a multi-material subframe that achieves a =25% weight reduction at an additional variable cost of =$4.27/lb of weight saved when compared to baseline stamped steel technology to be replaced.

4:20 PM
Benefits of Materials Modelling for Processing Simulation: *Zhanli Guo*[1]; [1]Sente Software Ltd
The validity of CAE simulation depends entirely on the availability of appropriate material data as input, which at present rely heavily on experimental measurements. Recent advancement in computational power enables such simulations to consider a multitude of physical phenomena as well as their interactions. Consequently the material data essential for such simulations have to cover a wide range, from physical and thermophysical properties, rheological properties to phase transformation kinetics. While it might be possible to have a spectrum of modelling tools which tackle a certain length scale before moving up to the next level, it would be more appealing to industry if the number of modelling tools needed can be reduced while providing a high quality simulation. This paper reviews the development of such a tool based on thermodynamics, phase transformation kinetics and microstructure-property relationships. Benefits of this approach in processing simulation are demonstrated in some case studies.

ICME 2019 — Linkage: Process-Microstructure II

Wednesday PM
July 24, 2019

Room: White River I-J
Location: JW Marriott Indianapolis

Session Chair: To Be Announced

2:00 PM
The PRISMS-PF Open-source High-performance Framework for Phase Field Modeling and Its Use in ICME Investigations of Mg Alloys: *Stephen Dewitt*[1]; David Montiel[1]; Katsuyo Thornton[1]; [1]University of Michigan
Phase field modeling plays an important role in the ICME paradigm with its capability to link processing to microstructure. General-purpose frameworks for phase field modeling have received increasing attention, promising decreased development time compared to traditional single-purpose codes. Here, we discuss PRISMS-PF, an open-source high-performance phase field modeling framework with a flexible and user-friendly interface for implementing new models. The use of a matrix-free finite element method with high-order elements, adaptive meshing, and multilevel parallelism enables strong computational performance. We demonstrate a marked reduction in run times compared to simulations using other open-source phase field frameworks as well as a finite difference code. We then discuss the use of PRISMS-PF in ICME investigations of precipitation in Mg-rare earth alloys. We show that phase field simulations are a vital link in a platform that also includes first-principles calculations, statistical mechanics methods, CALPHAD databases, dislocation dynamics simulations, and experiments.

2:20 PM
Development of a CALPHAD Based Steel Property Model Library for Martensite and Pearlite: *Paul Mason*[1]; Jiayi Yan[2]; Johan Jeppsson[2]; Qing Chen[2]; [1]Thermo-Calc Software Inc.; [2]Thermo-Calc Software AB
CALPHAD based tools are an important component of ICME since by combining thermodynamic and mobility data, kinetic reactions during solidification and heat treatment processes can be simulated. Extension of CALPHAD models to predict other properties is now being undertaken. Three examples are given for steels. A new Martensite Temperature property model calculates the martensite start temperature (Ms) based on modeling the transformation barrier with fitted analytical equations. The partitionless equilibrium temperature T0 is calculated using a CALPHAD database. The model also gives temperatures corresponding to 50%, 90%, and 99% transformations where Martensite fractions are based on the fraction of athermal martensite calculated using an analytical equation [Huyan et al. (2016)] A new Pearlite property model describes the thermodynamics and kinetics of pearlite formation from austenite. Growth rate and lamellar spacing of pearlite are determined by a criteria where either growth rate or Gibbs energy dissipation rate is maximized.

2:40 PM
A New Bimodal Microstructure Design for Improving Metal Fatigue: *Wenwu Xu*[1]; Ken Ramirez[1]; Rachell Lee[1]; Sharier Hasan[1]; [1]San Diego State University
This talk will provide an example of structure-property design of a new bimodal microstructure for improving metal fatigue using molecular dynamics (MD) simulations. In this bimodal microstructure, individual micrometer-sized grains are completely separated by a network of ultrafine nanocrystalline structure. MD simulations of low cycle fatigue deformation of the proposed bimodal microstructure suggest that most of the dislocations generated by the repeated plastic deformation are absorbed by the nanocrystalline network. No significant accumulation of dislocations is observed within the micrograins. The underlying mechanism is probably related to the intrinsic characteristic of nanograin boundaries. The excess volume (or the width) of nanograin boundaries in the nanocrystalline network changes reversely during the repeated compression and tension, impacting the dislocation behavior within micrograins. This work suggests a potential path to achieve high fatigue resistance in metals as compared with their microcrystalline counterparts, which would be useful in nearly every engineering setting.

3:00 PM
Predicting Twin Nucleation in a Polycrystalline Mg Alloy Using Machine Learning Methods: *Leyun Wang*[1]; Zhounuo Tong[1]; Gaoming Zhu[1]; Xiaoqin Zeng[1]; [1]Shanghai Jiao Tong University
Twinning is an important deformation mechanism for Mg alloys. So far, there is no satisfactory criterion to predict twin nucleation in a polycrystalline Mg alloy prior to its deformation. In this work, we employ the machine learning approach to tackle this problem. From a Mg-0.47wt%Ca extruded alloy, three tensile specimens of different orientations were fabricated. After 4% strain, twins were found in all three specimen. 18 attributes such as grain size and Schmid factors of different slip systems are computed for grains with or without twins. Five algorithms including decision tree, artificial neural network (ANN), support vector machine (SVM), Naïve Bayes, and Bayesian network are then used to build models to predict twin nucleation using one specimen as the training set and the other two specimens as test sets. The performance of different models are compared with each other in terms of accuracy and F1 metrics.

3:20 PM Break

3:40 PM
Microstructure Based Process Modeling and Integration of U-10%wt Mo Alloys: *Chao Wang*[1]; Zhijie Xu[1]; William Frazier[1]; Ayoub Soulami[1]; Saumyadeep Jana[1]; Kyoo Sil Choi[1]; Curt Lavender[1]; Vineet Joshi[1]; [1]Pacific Northwest National Laboratory
Low-enriched uranium alloyed with 10wt% molybdenum (U-10Mo) has been recognized as a promising candidate to replace high-enriched uranium fuel due to its ability to meet the neutron flux demands of U.S. high power research reactors and initial experimental evaluations of irradiation performance. Manufacturing the U-10Mo alloy involves a complex series of thermomechanical processing steps, including homogenization, hot rolling, annealing, cold rolling, and hot isostatic pressing. As part of this project, several models/modeling methods have been developed for the individual processes. The interaction and coupling between individual processes use the concept of ICME which aims to bridge the information passing between interacting models and investigates the impact of manufacturing processes on material microstructure evolution. The ICME framework is demonstrated by combining all the individual processes. It is shown that the implementation of ICME leads to improved predictions, better understanding of microstructure across multiple processes, and accelerated and more cost-effective development effort.

4:00 PM
Process-structure-properties-performance Modeling for Selective Laser Melting of 316L Stainless Steel: Anssi Laukkanen[1]; *Tatu Pinomaa*[1]; Tom Andersson[1]; Matti Lindroos[1]; Ivan Yaschuk[1]; [1]VTT Technical Research Centre of Finland
Selective laser melting (SLM) is a promising manufacturing technique to produce complex parts for biomedical and aerospace industry from 316L stainless steel. One of the challenges of SLM is to be able to predict the microstructural features that result from controllable process parameters, and how these microstructural features determine the mechanical properties and performance of the material. A large scale heat transfer model is first used to estimate the range of expected thermal gradients and cooling rates, which are then used to conduct directional phase field simulations to assemble a process-microstructure map based on thermal gradient and cooling rate. The cellular structures are analyzed with a micromechanical crystal plasticity model, to predict the properties and performance of the material, including material fatigue resistance.

4:20 PM

Modeling of Hydrogen Porosity Evolution and Dendritic Growth under Convection in Al-Cu Alloys: *Ang Zhang*[1]; Shaoxing Meng[1]; Zhipeng Guo[1]; Qigui Wang[2]; Shoumei Xiong[1]; [1]Tsinghua University; [2]General Motors

Microporosity is recognized as the most detrimental defect that can severely deteriorate the mechanical properties of solidified materials. Simulating the microporosity formation in castings is challenging due to large liquid-gas density ratio, complex topological morphology, and intricate interaction involving multi-physical field and multiphase. In this work, a 3D multiphase-field lattice-Boltzmann model is developed to simulate the growth, deformation and motion of hydrogen porosity during solidification of dendrites in Al-Cu alloys. Model validation is performed by simulating bubbles dynamics under different configurations, and good agreements are achieved between the simulation results and analytical solutions. To facilitate large-scale 3D simulations, a parallel-adaptive mesh refinement algorithm is employed to reduce the computing overhead. Porosity evolution coupled with dendritic growth under convection is characterized. Results show that the size, distribution, and initial hydrogen concentration of porosity have remarkable influence on the final microstructure, which compares reasonably well with the available experimental data.

4:40 PM

Phase-field-immersed Boundary-lattice Boltzmann Simulations of Dendrite Growth and Motion by Employing Para-AMR Algorithm: *Shaoxing Meng*[1]; Ang Zhang[1]; Zhipeng Guo[1]; [1]Tsinghua University

An immersed boundary lattice Boltzmann method (IB-LBM) coupled with phase-field model is developed to simulate the growth and motion of dendrites under convection. To maintain mass conservation, a conservative phase-field model, rather than convectional motion equation, is employed to characterize the dendritic motion. A parallel and adaptive mesh refinement (Para-AMR) numerical algorithm is developed to improve the computational efficiency. Numerical simulation results show the difference of dendrites growth with and without the dendritic motion and the multiple dendritic collision and coalescence. The interaction between dendrites and fluid is precisely described, which enables us to gain more information on dendrite under flow and to simulate the dendrite growth in actual solidification process.

ICME 2019 — Linkage: Structure-Properties II

Wednesday PM
July 24, 2019

Room: White River G-H
Location: JW Marriott Indianapolis

Session Chair: Qiang Feng, University of Science and Technology Beijing

2:00 PM

Damage Assessment and Remaining Creep Life Prediction for Serviced Turbine Blades Made of Directionally-solidified Nickel- base Superalloy by ICME Framework: Chao Fu[1]; Yadong Chen[1]; Siliang He[1]; Stoichko Antonov[1]; Longfei Li[1]; *Weiwei Zheng*[1]; Qiang Feng[1]; [1]University of Science and Technology Beijing

An ICME framework for predicting the remaining creep life of serviced turbine blades made of a directionally solidified (DS) superalloys was developed by considering micro and macro criteria. This framework comprises of four capabilities, i.e., quantitative microstructural characterization, service condition assessment, degradation evaluation and remaining creep life prediction, using artificial neural network models and a modified θ projection model based on quantitative microstructural evolution datasets of the DS superalloy obtained by high-throughput thermo-mechanical creep testing and systematic analysis of the corresponding creep curves under different conditions. Through this ICME framework, the damage levels of two serviced turbine blades, after different service periods, were assessed and the remaining creep lives were predicted. The results were verified by creep tests using miniature samples cut from serviced blades. The development of this new framework provides a reference in the design and service evaluation of turbine blades made of Ni-base superalloy.

2:20 PM

A Multi-scale Characterization of Strain Localization in Ni-based Superalloys – Combined HEDM and Dark Field X-ray Microscopy: *Sven Gustafson*[1]; Wolfgang Ludwig[2]; Paul Shade[3]; Diwakar Naragani[1]; Darren Pagan[4]; Michael Sangid[1]; [1]Purdue University; [2]European Synchrotron Radiation Facility; [3]Air Force Research Laboratory; [4]Cornell High Energy Synchrotron Source

Fatigue is naturally a multi-scale phenomenon. To predict crack initiation, models are informed and validated by multi-scale characterizations which probe the intragranular strain due to crystallographic slip, a catalyst for crack initiation. In this work, a multi-scale characterization is presented of a polycrystalline Ni-based superalloy subjected to fatigue loading. High energy x-ray diffraction microscopy (HEDM) was used to study the microstructure and evolution of the grain averaged lattice strains during loading. Afterwards, a grain of interest was selected and extracted for additional investigation. Dark field x-ray microscopy, which magnifies the diffracted image from a thin region while motors rock the sample through diffraction space, was completed on the sample to directly measure the intragranular orientation within the grain with 200nm resolution, enabling the visualization of lattice deformation within the grain of interest. The presented preliminary results represent a step forward in multi-scale characterization to identify cyclic deformation and strain localization.

2:40 PM

Data Assimilation for Fatigue Life Prediction of Welded Joint: *Takayuki Shiraiwa*[1]; Manabu Enoki[1]; [1]University of Tokyo

Fatigue life of welded joint is complicatedly affected by various factors such as geometries, defects, residual stress and microstructure. In our previous research, a numerical framework for fatigue life prediction of welded joints has been developed by integrating several computational techniques including welding simulation, crack initiation analysis with crystal plasticity finite element method, and crack growth analysis with extended finite element method. Although the predicted fatigue life showed good agreement with the experimental data, it requires significant time to calibrate model parameters by trial and error. The purpose of this study is to propose a novel approach to estimate model parameters related to fatigue life prediction more efficiently by data assimilation method. As an example, the heat source parameter in the welding simulation was estimated from experimental data by Bayesian optimization. Also the effects of the selection of acquisition function and objective function on the calculation cost were evaluated.

3:00 PM

Yield Surface Prediction by Virtual Microstructure and Testing: *Junhe Lian*[1]; Wenqi Liu[2]; Fuhui Shen[2]; Sebastian Muenstermann[2]; [1]Aalto University; [2]RWTH Aachen University

The powerful mechanism of the multiscale modelling lies in the construction of a representative virtual microstructure model allowing consideration of the relevant material parameters and a virtual testing scheme bridging the equivalent quantities from microstructure to macroscopic level. In this study, we firstly aim to give an overview of various virtual microstructures with respects to the application of metals. The capability and limitation of these models to describe the comprehensive microstructure features are discussed. Secondly, we aim to give application examples incorporating such a multiscale modelling approach relying on the virtual microstructure and testing to correlate the microstructure to the yield surface for various metals. The focuses are on i) the construction a specific virtual testing scheme for a robust prediction and upscaling of the microstructural-level data to the macroscopic phenomenological yield criteria and ii) the viscoplastic behavior of materials and the prediction of it by crystal plasticity models.

3:20 PM Break

3:40 PM
Phase Field Modeling of the Effect of Microstructure during the Corrosion of Alloys: *David Montiel*[1]; Stephen DeWitt[1]; Katsuyo Thornton[1]; [1]University of Michigan
We apply the phase field and smoothed boundary methods to study the role of microstructure on the propagation of the corrosion front into the material during nominally uniform corrosion in Mg-RE alloys. We employ multiple order parameters to represent grains and precipitates in a polycrystalline metal and a liquid electrolyte. The evolution of these order parameters is coupled to the evolution of the concentration of ionic species and electrostatic potential in the electrolyte and the interfacial electrochemical reaction rate. In the course of this work, we developed a new application within the PRISMS-PF open-source phase field modeling framework. A new hybrid Newton-Picard nonlinear solver was added to PRISMS-PF to obtain the electrostatic potential and to integrate the time-dependent equations under an implicit Euler time discretization scheme. We show how the size and distribution of precipitates affects corrosion rate and the geometry of the corrosion front.

4:00 PM
Materials Margins Assurance: Incorporating Material Variability in Simulation Tools & Code: *Jonathan Madison*[1]; Theron Rodgers[1]; Hojun Lim[1]; Kyle Karlson[1]; John Mitchell[1]; Corbett Battaile[1]; Alyssa Skulborstad[1]; Maher Salloum[1]; Alex Hanson[1]; John Emery[1]; [1]Sandia National Laboratories
Performance in engineering components can vary widely based on several factors including processing anomalies, defect presence and any number of design decisions accompanying the product. In most cases, mitigation strategies against property shortfalls take the form of safety factors or over-design relative to anticipated loads. However, these approaches do little to account for, or provide insight to, performance changes owed to material variability itself. To address this gap, the Sandia Materials Margins Assurance Program was erected and will be presented in the context of work performed on challenges having impact to high consequence applications. In this talk, three exemplar problems will be featured; (1) microstructural predictions in additive materials, (2) grain scale deformation in micro-springs and (3) ductile failure in laser welds. Each exemplar will be accompanied by a corresponding approach to meaningfully incorporate a particular type of material variability in simulation tools to better understand ensemble performance.

4:20 PM
Modeling J2 Plasticity and Crystal Plasticity in a Unified Time-dependent Ginzburg-Landau Framework: *Tianle Cheng*[1]; Youhai Wen[2]; Jeffrey Hawk[2]; [1]National Energy Technology Laboratory / AECOM; [2]National Energy Technology Laboratory
By taking traceless inelastic strain as a phase field variable and minimizing the total elastic energy through constrained variational method, the kinetics derived from the time-dependent Ginzburg-Landau (TDGL) type equation can recover J2 type viscoplasticity and crystal plasticity flow rules. Based on this framework, a polycrystal plasticity model has been developed that can accommodate grain boundary sliding (GBS), an important deformation mechanism for metals and ceramics at high temperatures. The grain structure in this polycrystal plasticity model is extracted directly from phase-field grain growth simulations rather than from the commonly used Voronoi tessellation. The model is validated against analytical solutions and the finite element simulation results of Crossman & Ashby and Ghahremani on GBS.

4:40 PM
Studying the Effect of Dopants on Properties of Lightweight Materials with Atomistic Simulations: *Shengfeng Yang*[1]; [1]Indiana University; Purdue University Indianapolis
The properties of lightweight materials can be improved through doping. In this study, atomistic simulations are used to study the deformation mechanisms of nanocrystalline aluminum alloys and magnesium alloys and investigate the effect of dopants on their properties. Hybrid Monte Carlo and molecular dynamic simulations were used to achieve both mechanical and chemical equilibrium in nanocrystalline materials. The simulation results of tensile testing show an improved strength, including the yield strength and ultimate strength, through doping 5 at.% Mg into nanocrystalline aluminum. The results of atomic structures clearly reveal the multiple strengthening mechanisms related to doping in Al-Mg alloys. At the early deformation stage, the strengthening mechanism of dopants exhibits as dopant pinning grain boundary (GB) migration. At the late deformation stage, which is close to failure of nanocrystalline materials, dopants can prohibit the initiation and propagation of intergranular cracks and thus improving the flow stress of Al-Mg alloy.

ICME 2019 — Application: Additive Manufacturing II - Composition

Thursday AM
July 25, 2019

Room: White River F
Location: JW Marriott Indianapolis

Session Chair: To Be Announced

8:00 AM Invited
CALPHAD-based ICME Design for Additive Manufacturing: Success and Challenges: *Wei Xiong*[1]; Albert To[1]; Yunhao Zhao[1]; Xin Wang[1]; Qian Chen[1]; [1]University of Pittsburgh
Phase transformations in laser melting can readily influence the mechanical properties of the 3D printed components. An effective ICME simulation with a reliable prediction of phase transformations becomes essential, and can significantly help additive manufacturing design with lower costs and reduced development cycles. In this talk, we discuss two cases by applying the CALPHAD approach for powder-bed laser melting simulation and steel powder composition design. A CALPHAD-based ICME framework is established using CALPHAD-informed thermal modeling, CALPHAD and finite element coupled phase transformation, mean-field type simulation for post-processing design. The case studies on Inconel 718 and HSLA (High-strength low-alloy) steels demonstrate the effectiveness of such a design framework. In addition, knowledge gaps are identified using the case studies, supporting metallurgical experiments for model calibration and improvement are essential for the successful ICME design. The established ICME design framework demonstrated the collaborative efforts made by mechanical engineering and materials science for additive manufacturing modeling.

8:20 AM
A Parametric Study on the Role of Composition on Process-induced Voids during Additive Manufacture of Nickel-based Superalloys: *Lucia Scotti*[1]; Magnus Anderson[1]; Ben Sauders[2]; Hector Basoalto[1]; [1]University of Birmingham; [2]Rolls-Royce plc
The additive manufacture (AM) of nickel-based superalloys is characterised by significant variations of process-induced microstructures, which result in variable property scatter of AM parts. The formation of microvoids in these alloys has complex dependencies on the details of the melt-pool behaviour and processing scanning strategy used. Understanding these dependencies is key in the determination of optimum process parameters seeking minimise process variability. This work presents a multiscale materials modelling framework for simulating the melt-pool evolution, solidification porosity/voids and grain structures. The approach is based on a volume of fluids formulation for simulation of the melt-pool, where composition is explicitly taken into account. The discrete element method is used to generate the powder dispersions. Predictions of the microvoid distributions for IN625, IN718 and CM247LC will be presented as a function of process conditions (power and scanning speed) as well as the influence of heat source models on process-induced void distributions.

8:40 AM

Rationalisation of Vapourisation during Powder Bed Fusion Additive Manufacturing in Nitinol and Nickel-based Superalloys: *Chinnapat Panwisawas*[1]; [1]University of Oxford

Mass loss due to vapourisation induced by the high energy heat source during powder bed fusion additive manufacturing (AM) is a central issue which concerns the compositional homogeneity across the additively manufactured build. Chemical species impairing from the anticipated recipe allow sensitive area where defects can be initiated. In this work, evaporation effect of powder bed fusion AM in Nitinol (NiTi) and nickel-based superalloys is studied via physics-based integrated modelling framework and experimental investigation. Volatile species which depart from the nominal composition result in significant mass lost up to 2 atomic percent of Ni in the binary alloy system Nitinol, consistent with energy-dispersive X-ray analysis. As for the multicomponent alloy system in nickel-based superalloys, modelling results reveal further that Al, Cr and Fe are preferable to vaporise first, backed by chemical analysis. Hierarchical microstructures have been characterised to rationalise the process-structure-property relationship.

9:00 AM

Phase Field Simulations of Delta Phase Precipitation during Annealing of Additively Processed Alloy 625: *Bala Radhakrishnan*[1]; Sarma Gorti[1]; Lyle Levine[2]; John Turner[1]; [1]Oak Ridge National Laboratory; [2]National Institute of Standards and Technology

It is known that during laser bed powder fusion experiments in alloy 625, gamma" and delta phases precipitate during post-process stress relief anneal. The objective of this talk is to demonstrate this co-precipitation process using phase field simulations, taking into account the thermodynamics of the alloy, the AM process induced segregation of alloying elements, the presence of inter-dendritic boundaries, and the effect of elastic energy during solid-state precipitation. The simulations will be first validated using process data generated as part of the NIST AM-Bench experiments. The validated code will then be used to identify the effect of temperature and time on gamma" and delta co-precipitation during stress-relief anneal. Full 3d simulations with high spatial resolution will be performed taking advantage of the high performance computing resources at the Oak Ridge National Laboratory through the Exascale Computing Project and the Oak Ridge Leadership Computing Facility under contract DE-AC05-00OR22725.

9:20 AM

The Effects of Process Parameters on the Thermal History and Mechanical Behavior of Laser Powder Bed Fused 17-4 PH Stainless Steel: Mohammad Masoomi[1]; *Yi Zhang*[1]; Rakish Shrestha[2]; Nima Shamsaei[2]; Jeff Burdick[1]; [1]Ansys, Inc.; [2]Department of Mechanical Engineering, Auburn University

The microstructure and mechanical response of additively manufactured parts are affected by the thermal history experienced, which in turn is a function of design parameters as well as manufacturing process parameters. In this study, a thermal simulation approach is proposed based on ANSYS software to better understand the effects of the process parameters on the mechanical response for laser-powder bed fusion processes. Accordingly, the effect of process parameters on resulting thermal history, porosity, and mechanical properties of L-PBF 17-4 PH stainless steel is investigated employing a systematic experimental-computational approach. First, four parts with different process parameters are designed and fabricated. The process parameters are proposed with the help of ANSYS Additive Science to ensure full density of the parts. ANSYS software is used to simulate thermal histories for each part to predict their variations. Finally, the parts are fabricated, and mechanical testing is done to validate the simulation results.

9:40 AM

CALPHAD-based Sensitivity Analysis in Powder Composition Design for 3D Printing: *Xin Wang*[1]; Wei Xiong[1]; [1]University of Pittsburgh

During the powder manufacturing of metals 3D printing, the practical composition will deviate from the designed composition, which may lead to the undesired property of printed alloy. It is critical to perform the sensitivity analysis during the ICME compositional design to identify the proper composition range that meets property requirements. In this work, a high-throughput sensitivity analysis was performed by using the CALPHAD-based process-microstructure models with 10,000 compositions near the High-strength Low-alloy (HSLA)-115 steel composition. The required properties, such as critical transition temperatures, phase fractions, are calculated. The new average composition and its manufacturing uncertainty range with less detrimental phases and more desired strengthening precipitates are determined. It shows a higher probability of meeting all the requirements than the one defined empirically. The present study provides a strategy to efficiently optimize the alloy composition for additive manufacturing powder production, and it can be further extended for powder composition design.

10:00 AM Break

ICME 2019 — Multi-scale Modeling Developments

Thursday AM
July 25, 2019

Room: White River I-J
Location: JW Marriott Indianapolis

Session Chair: To Be Announced

8:00 AM

Stochastic Multiscale Modeling of Random Structures: *Mujan Seif*[1]; Skylar Mays[1]; Katherine Moody[1]; Matthew Beck[1]; [1]University of Kentucky

Increasingly, engineers are seeking to design and fabricate materials with properties and functions driven by complex, even inherently random, intrinsic structures. These materials include nanoporous materials, ablatives, membranes, 3D printed metals, and biomaterials. Despite the potential impact of these materials, computational limitations for modeling randomness have hindered development of predictive tools and required imprecise simplifications to homogeneous, ordered structures. Here, we present a stochastic modeling approach for the high-throughput assessment of random structures. We demonstrate a highly flexible algorithm for building large numbers of representative volume elements (RVEs), which are based on a user-defined "seed" geometry and then modified to allow for the systematic study of specific geometric/structural factors (e.g. coordination, area of contact, reduced density) of interest. With subsequent finite element analysis, the behavior of the RVE's can be extensively evaluated, providing insight into the magnitude and variation of the properties of randomly structured materials.

8:20 AM

Modeling and Simulating Defects in Ionic Materials with a Concurrent Atomistic and Continuum Method: *Shengfeng Yang*[1]; [1]Indiana University; Purdue University Indianapolis

The behavior of defects such as dislocations, cracks and grain boundaries in ionic materials is modeled and simulated by a concurrently coupled atomistic and continuum methodology (CAC). This methodology provides a seamless interface between atomistic and continuum region through combining a new formalism of balance laws and a modified Finite Element method. The defects such as crack and dislocation can naturally pass the atomic-continuum interface without any empirical rules or additional techniques. In CAC, the critical regions near defects are modeled atomistically, and the regions away from defects are modeled with coarse elements. CAC is used to simulate the evolution of defects when interacting with other defects in ionic materials like strontium titanate. The effect of cracks, dislocations, grain boundaries and the interactions between them on the structure and properties of materials are studied.

8:40 AM

Bond-order Model for Bond Energies in Alloys: *Wolfgang Windl*[1]; Szu-Chia Chien[1]; Christian Oberdorfer[1]; [1]Ohio State University

Thermodynamic modeling of alloys requires the ability to determine the energy of the different atoms in the alloy, which traditionally has been a drawback of first-principles calculations where the energy is typically only known for the entire system, but not for the different atoms. One of the oldest approaches to determine such atomic energies is the quasichemical solution theory (QST), where bond energies are assigned to the different bond types. However, QST has at times been labeled as a "naïve theory" and not rigorous, and more complicated approaches with increased numbers of parameters have been developed, most notably the cluster expansion. Here, we will show that introducing appropriate bond-order functions to establish a bond-order model for bond energies can result in models that provide high quality energy fits and can even span different crystal structures such as face-centered cubic and body-centered cubic. Application examples go from binary to high-entropy alloys.

9:00 AM

A Smoothed Particle Hydrodynamics (SPH) Procedure for Simulating Cold Spray Process - An Additive Manufacturing Process without Heat Supply: *Balachander Gnanasekaran*[1]; G R Liu[1]; Yao Fu[1]; Guangyu Wang[2]; Weilong Niu[1]; Tao Lin[1]; [1]University Of Cincinnati; [2]Nanjing University of Science and Technology

Cold spray process has been of great interest in coating and additive manufacturing because it does not need heat supply during impact. Cold spray generally uses particles of diameters 10\181m to 50\181m traveling at velocities of 300m/s to 1200m/s, and it takes place at very small time and length scales. Thus, it becomes difficult to observe the detailed process experimentally. The feature of Smoothed Particle Hydrodynamics as a tool for modeling large deformation well poses an important advantage for its usage in the simulation of cold spray process, and hence it is adopted in this study. Our SPH model includes failure modeling for copper particle impacts. It was found that larger particles had greater bonding ability and an impact angle between 80\176 and 90\176 is conducive for bonding. Finally, our SPH procedure is extended to simulate three-dimensional cold spray problems with multiple particles.

9:20 AM

Genome-based Multiscale Modeling of Crack Formation during Laser Directed Energy Deposition of Alumina Ceramics: *Xiangyang Dong*[1]; [1]Missouri University of Science and Technology

Laser directed energy deposition (L-DED), one of the additive manufacturing (AM) techniques, is a promising process capable of rapidly fabricating ceramic components with controllable microstructure. However, crack control poses one major challenge in L-DED of ceramics and limits its applicability. In this study, a multiscale genome framework is developed to model the complex cracking patterns within additively manufactured alumina ceramics. A combined phase field-cohesive zone model is embedded in the formulation of the multiscale genome through the variational asymptotic method for unit cell homogenization. The genome modeling is shown to greatly reduce the computational costs in predicting the relationship between microstructure and cracking. The study investigates the influence of deposition conditions on crack patterns. The developed model captures the typical characteristic of crack formation within deposited alumina ceramics. It is also found that the composition and interfacial phase play a major role in cracking during L-DED of alumina ceramics.

9:40 AM

A Lattice BGK Method for Modeling of Liquid-solid Phase Transition with Melt Convection: *Dongke Sun*[1]; Rui Du[1]; [1]Southeast University

A lattice Bhatnagar-Gross-Krook method is proposed to study phase transition of alloys with melt convection. It extends the BGK-Boltzmann equation to model the heat transfer, melt convection and liquid-solid phase transition by implementing a general streaming-relaxation steps based on the Chapman-Enskog expansion. Three sets of distribution function are adopted to describe the evolution of the temperature, flow and phase fields. The DnQd lattice vectors are used to describe advancement of solid-liquid interface, coupling with a convective-diffusion equation for heat transfer during solidification. It offers a simple and effective geometrical relationship between growing velocity and lattice spaces. After model validation, the liquid-solid phase transition of alloys with melt convection have been investigated numerically. The results show that the present model provides an alternative numerical approach to study solidification of alloys with relatively fast efficiency, and it would like to facilitate the understanding the features of phase transition in a high-throughput way.

10:00 AM Break

ICME 2019 — Uncertainty Quantification and Validation

Thursday AM
July 25, 2019

Room: White River G-H
Location: JW Marriott Indianapolis

Session Chair: Deborah Mies, Granta Design, ANSYS

8:00 AM

AM-Bench, A Set of Controlled Benchmarks for Additive Manufacturing: Lyle Levine[1]; *John Turner*[2]; Brandon Lane[1]; [1]National Institute of Standards and Technology; [2]UT-Battelle / Oak Ridge National Laboratory

Additive manufacturing (AM) of metal components is undergoing rapid adoption due in part to the ability to produce geometrically complex parts. However, extreme processing conditions create location-dependent microstructures, properties, and residual stresses that complicate component and process certification. Quantitative modeling of these characteristics is critical, but model validation requires rigorous measurements including comprehensive in situ monitoring of melt pool behavior, along with microstructure, residual stress, and property characterizations. There is an increasing need for benchmark measurements that are broadly accepted by the international AM community, which will enable meaningful comparisons between simulations (approaches, models, and implementations). We describe the Additive Manufacturing Benchmark Test Series (AM-Bench), a continuing series of highly controlled tests that modelers around the world are using to test their simulations.This work was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.

8:20 AM

Online Tools for Calibration and Uncertainty Quantification in nanoHUB: *Saaketh Desai*[1]; Martin Hunt[1]; Alejandro Strachan[1]; [1]Purdue University

The use of mathematical models and simulation tools in ICME applications relies on rigorous uncertainty quantification (UQ) and propagation of uncertainties from model inputs to outputs. We will discuss the integration of the PRISM Uncertainty Quantification (PUQ) code with the nanoHUB infrastructure for simulations to enable automatic UQ in deterministic tools. This feature provides users with posterior distributions on output quantities, surrogate models and a sensitivity analysis of all tool inputs, given prior distributions on tool inputs. We also demonstrate an online tool that performs deterministic and Bayesian calibration for nanoHUB tools, in conjunction with the DAKOTA software package, to estimate calibrated posterior distributions for input quantities using surrogate models for tools generated using prior input distributions and reference outputs (with errors). We compare calibration results from using the generalized polynomial chaos surrogate model of the PUQ framework and the gaussian process surrogate model from the DAKOTA software package and demonstrate the improved prediction capabilities of calibrated tools in comparison with experimental data.

8:40 AM

CALPHAD in the Cloud – Webware and Framework for Uncertainty Quantification: *Changning Niu*[1]; Abhinav Saboo[1]; Ramon Frey[1]; Meng Li[2]; Jiadong Gong[1]; [1]QuesTek Innovations LLC; [2]Rice University

QuesTek has applied its expertise in ICME and CALPHAD to develop web-based tools for performing chemical thermodynamics calculations and for working with CALPHAD databases. A python-based web application for CALPHAD calculations using the Thermo-Calc software platform in combination with MySQL databases is developed at QuesTek and will be introduced. We also develop a Bayesian framework for incorporating uncertainty quantification into CALPHAD model databases and propagating this uncertainty through chemical thermodynamic calculations to provide credible intervals on predicted thermo-chemical quantities.

9:00 AM
Efficient Uncertainty Quantification and Propagation Workflows in ICME: *Gary Whelan*[1]; David McDowell[1]; [1]Georgia Institute of Technology
Uncertainty is intrinsically tied to decision-making in design. We consider hierarchical mapping of linkages between processing, structure, and properties of Ti64 with a range of microstructures. Each PS and SP linkage has uncertainty associated with it, arising both from the types of models or interpretation of experimental results used to form linkages, as well as model parameters. These uncertainties can propagate and significantly affect the decision making process in design of materials for ranged sets of goals. Uncertainty quantification can be a highly computationally expensive undertaking in materials design. In the current work, efficient protocols are developed to quantify these uncertainties and propagate them to investigate their effects of the rare-event high-cycle fatigue response of Ti64.

9:20 AM
Functional Uncertainty Quantification for Molecular Dynamics: Alejandro Strachan[1]; *Samuel Reeve*[1]; [1]Purdue University
Functional uncertainty quantification (FunUQ) was recently proposed to quantify uncertainties in models and simulations that originate from input functions, as opposed to parameters. This talk will review the approach and a computationally inexpensive expression to compute functional derivatives in MD derived from perturbation theory. We show that functional derivatives of the quantities of interest (average internal energy, pressure, and volume, for example) with respect to the interatomic potential can be used to predict those quantities for a different interatomic potential, without re-running the simulation. To facilitate reproducibility and to simplify the use of the approach, we created Jupyter notebooks to perform FunUQ analysis on MD simulations and made them available for online simulation in nanoHUB (as well as making the codes freely available for download). Finally, we will discuss the application of FunUQ in other materials modeling methods and its place within an ICME ecosystem.

9:40 AM
Uncertainty Quantification of Machine Learning Potential: *Yumeng Li*[1]; Xin Chen[1]; [1]University of Illinois at Urbana-Champaign
This paper is to investigate the uncertainty of machine learning potential associated with the employed atomic structure descriptors, the traning process and adopted neural network structures. Molecualr dynamics (MD) simulations are growing in importance in the material analysis and design with its first-principle accurary. The conventional physical force field potentials have large limitations due to their simplfied analytical formulations. Machine learning techniques have been explored for developing interatomic potentials to interpolate the potential energy surface for highly complex potential energy surface where empirical physical potentials may fail. The successful application of the machine learning techniques require a thourough uncertainty quantification to ensure their fadility. In this research, the Behler–Parrinello (B-P) approach based on high dimensional ANNs potential is employed for the development of machine learning potentials whereas the hign dimensional model representation (HDMR) based technique is employed for efficient uncertainty analsysis towards a case study of titanium dioxide (TiO2).

10:00 AM Break

ICME 2019 — Mesoscale Modeling of Metallic Systems

Thursday AM
July 25, 2019

Room: White River F
Location: JW Marriott Indianapolis

Session Chair: Charles Fisher, Naval Surface Warfare Center - Carderock

10:30 AM Plenary
Applications of CALPHAD Modeling and Integrated Computational Materials Engineering in Advanced Lightweight Metallic Materials: *Alan Luo*[1]; [1]Ohio State University
This talk presents an overview on the application of CALPHAD (CALculation of Phase Diagrams) modeling and integrated computational materials engineering (ICME) in the design and development of advanced lightweight metallic materials including magnesium, aluminum, titanium, aluminum-based metal matrix composites, and high entropy alloys. CALPHAD methodology has been established and summarized from the construction of databases describing thermodynamics, atomic mobility, kinetics, thermo-physical properties (such as viscosity) to the application of computational design of lightweight materials. The examples in this talk have demonstrated the effectiveness and capability of CALPHAD methodology in accelerating the design of lightweight materials by optimizing the compositions and various heat-treatment conditions, modifying the evolution of microstructures during processing, and finally predicting the mechanical properties (e.g., yield strength and hardness) of the lightweight components. Although the examples are given in lightweight alloys for structural applications, the fundamental methodology and modeling principles are applicable to all materials and engineering applications.

11:10 AM Plenary
Understanding, Prediction and Design of Mesoscale Structures and Properties of Functional Materials Guided by Phase-field Simulation: *Long-Qing Chen*[1]; [1]Pennsylvania State University
Phase-field method has thus far primarily been employed to reproduce and understand the evolution of experimentally observed materials microstructures or to test analytical theories. In order to establish phase-field method as a truly useful tool for ICME, there is a need to shift from purely "reproducing and understanding experimental observations" to "predicting mesoscale microstructures" and "guiding the synthesis and processing of materials to design their optimum properties and performances". This presentation will discuss a few examples on our recent attempts to employ the phase-field method to not only interpret experimental observations but also to provide guidance to experimental synthesis to achieve desirable mesoscale microstructures for optimum properties in functional materials. Examples include the discovery of novel polar states in ferroelectric superlattices and design of ultrahigh piezoelectricity in ferroelectric relaxor ceramics and single crystals guided by phase-field simulations and microstructure optimization for maximizing breakdown strengths of dielectric polymer composites.

11:50 AM Concluding Comments

ICME 2019 — Poster Session

Tuesday PM
July 23, 2019

Room: White Fiver F-J Foyer
Location: JW Marriott Indianapolis

Session Chair: Danielle Cote, Worcester Polytechnic Institute

3D Modeling of Fracture of Brittle Granular Materials: *Francois Guillet*[1]; Emile Renner[1]; Rafael Estevez[2]; Aurélien Doitrand[2]; [1]CEA; [2]Université Grenoble Alpes

Fracture of brittle polycristalline materials is governed by critical defects. Dispersion in size and nature of these defects lead to a dispersion of the critical stress that a given part may withstand before fracture. It is important in the context of defining a safe zone of operation for parts to accurately describe the failure probability for a given stress. This problem is even more critical for materials subjected to slow crack growth, for which propagation of cracks (and therefore part failure) may occur even when subcritical stresses are applied. This study is devoted to the (3D) modeling of fracture for such materials. The modeling of the fracture of a polycristalline material is carried out considering the Finite Elements Method with Cohesive Zones (CZ) inserted along the grain boundaries. The model, previously successfully developed in 2D [3], is currently under development for 3D; first results will be shown and discussed.

A Hierarchical Model to Simulate the Phase Transformation in AM Building and Post-processing: *Shengyen Li*[1]; [1]Southwest Research Institute

Selective laser melting additive manufacturing uses a small laser spot and high laser intensity to fuse metallic powder into a net-shape product in a layer-by-layer process. The as-built microstructure may contain a non-homogeneous composition distribution, high residual energy, and excessive void density, which creates microstructures distinct from traditional casting. In this work, the classic models including Scheil-Gulliver, diffusionless, densification and diffusion controlled models are reviewed and integrated to simulate the phase transformation during AM building and post-processing treatments for Ti-6Al-4V. This simulation model achieves tool maturity level 2 (TML-2), meaning it is capable of ranking or trending for a qualitative comparison to experimental results. The application space is clearly defined and the reference data is archived in Materials Data Curation System. The model sensitivity analyses will also be performed for the following model validation. A comparison of the predicted phase transformations to experimental observations will be presented.

A Modelling Based Approach towards Realizing Perovskite Solar Cells: *Jayita Dutta*[1]; Satyesh Yadav[2]; Sriram Goverapet Srinivasan[1]; Deepak Jain[1]; Parijat Deshpande[1]; Beena Rai[1]; [1]TCS Research; [2]Indian Institute of Technology, Madras

Perovskite materials with ABX_3 chemistries are highly hydrophilic and unstable in nature as compared to mixed halide perovskites. This paper describes the implementation of statistical learning methods using SVM based classifier with elemental features/descriptors to predict formability, followed by DFT approach to study structural and electronic properties of select mixed-halide/ion-doped $ABX_{(3-x)}Y_x$ perovskite chemistries. Predicted $CH_3NH_3PbI_3$ perovskite incorporating thiocyanate $(SCN)^-$ ions with formation probability of 94% are analyzed via DFT calculations since incorporation of $(SCN)^-$ is reported to improve moisture stability and perovskite film morphology. DFT calculations using plane-wave basis set, PAW pseudopotentials, PBE-GGA method, to rank suitability as a photovoltaic candidate, is conducted on a 2 × 2 supercell of $CH_3NH_3PbI_{(3-x)}(SCN)_x$ based stoichiometry using VASP® package with increasing % of $(SCN)^-$ in steps of 0,16,32,48% and corresponding % decrease of I^- in the perovskite composition. Subsequently, these short-listed perovskite chemistries are synthesized and tested for solar cell applications.

A Study of ICME and Intelligent Manufacturing for Complex Nickel-based Superalloy Castings: *Donghong Wang*[1]; Da Shu[1]; Haijun Huang[1]; Anping Dong[1]; Baode Sun[1]; Guoliang Zhu[1]; [1]Shanghai Jiao Tong University

A new cast polycrystalline nickel based superalloy was designed by the high-throughput composition design and calculation method. Taking grain sizes and the porosity indexes as input parameters, and tensile strengths, elongations and fatigue lives as output parameters, the relationship among microstructure, defect and mechanical properties was constructed by using a multi-scale calculation. A novel high-throughput method for establishing the solidification-microstructure relationship is presented. In addition, the artificial intelligence algorithm was used to optimize the shrinkage defect and the casting yield. The obtained result is suitable for both the laboratory and industrial applications.

Accurate Simulation of Complex Temperature Field in Aluminum Alloy Counter-pressure Casting Process: Yuncan Tian[1]; *Bo He*[1]; [1]Shanghai University of Engineering Science

In this study, dynamic thermomechanical analysis, differential scanning calorimetry, laser flash method and other methods were used to study the thermos-physical properties of AlSi7Mg, a physical model of counter-pressure casting system, including tooling and aluminum inside, was established based on the combination of the tested properties and database ones of aluminum, with the consideration of the presence of including, rare earth and rapid solidification. The temperature field of the system was computed and verified by thermocouples at six different points in tooling and the shrinkage simulation. It is found that the plot shape of computed temperatures and measured ones fit each other perfectly, and the difference between the peaks and valleys are controlled in 3% average, and 7% maximum in only one point, and the shrinkages predicted are all verified in the casting. This study is a solid foundation of future simulation, such as solution and morphologies of the microstructure.

Achieving Large Volume Grain Statistics with X-ray Diffraction Contrast Tomography: *Hrishikesh Bale*[1]; William Harris[1]; Erik Lauridsen[2]; Nicolas Gueninchault[2]; Jun Sun[2]; [1]Carl Zeiss X-ray Microscopy; [2]Xnovo Technology

An integrated microstructural modeling approach, and ensuring the handshake between modeling and experimentation, relies on adequate experimental statistics. Furthermore, recent simultaneous improvements in computing power and characterization techniques have opened up new possibilities in 4D analysis, beyond established 2D microstructural methods. Here we present the X-ray based technique of diffraction contrast tomography performed on a laboratory X-ray microscope. The LabDCT technique produces 3D grain maps over large volumes of material (upwards of 8 mm3) containing hundreds to thousands of grains in a matter of hours. Such experimental data is valuable either for validation or as input volumes for simulation. Moreover, with its nondestructive nature, LabDCT enables tracking the structural evolution through processes such as annealing or grain growth, addressing the essential needs of analogous models for experimental evidence. The technique and examples will be presented to highlight the acquisition of experimental datasets including necessary large statistics and dynamic evolution.

Advanced Processing and Visualization of 3D EBSD/EDS Experimental Data: *Laurie Palasse*[1]; Daniel Goran[1]; [1]Bruker Nano GmbH

A lot of effort is put into efficiently designing and engineering new materials and improving manufacturing processes via computational method. However, their validation can only be done by 2D and 3D microstructure characterization using experimental data. 3D electron backscatter diffraction(EBSD) measurements are required to get the complete crystallographic characterization of interfaces, morphology and orientation. This analytical technique brings the most advanced 3D insights into the deformation mechanisms of materials and enables experimental and theoretical crystal plasticity studies [1]. 3D EBSD/EDS is a destructive tomographic method consisting of repeated sectioning and subsequent characterization by EBSD and simultaneous elemental analysis by EDS. The measured database is later reconstructed and visualized with dedicated software. To this aim, ESPRIT QUBE was developed as a unique quaternion-based software that enables true 3D data representation and analysis. We will review ESPRIT QUBE 3D capabilities including slice realignment, data filtering, GND calculation [2], grain reconstruction and subsetting. References: [1] Zaefferer, S. et al. (2009) Three-Dimensional Orientation Microscopy by Serial Sectioning and EBSD-Based Orientation Mapping in a FIB-SEM, in Electron Backscatter Diffraction in Materials Science,A.J. Schwartz,et al.,Chapter 3,109-122.[2] Konijnenberg P., et al. (2015). Assessment of geometrically necessary dislocation levels derived by 3D EBSD, Acta Materialia, 99, 402-414.

Calculation of Phase Equilibria in Ti–Al–Cr–V-Nb System for Developing High Entropy Alloys: *Ker-Chang Hsieh*[1]; Tong You Liou[1]; Chia Ju Huang[1]; Shian-Ching Jang[2]; [1]Department of Materials and Optoelectronic Science, National Sun Yat-Sen University; [2]Department of Mechanical Engineering, National Central University

The Ti–Al–Cr–V-Nb system is a potentially useful system for developing medium weight high entropy alloys; however, there are few reports about the experimental phase diagrams and the thermodynamical assessment for this system. In this study, the previous investigations for the thermodynamic descriptions of the ternary subsystems in the Ti–Al–Cr–V-Nb system are reviewed, and some of the previous assessment for the related ternary sub-systems in this quinary system is summarized, the thermodynamical database of this quinary system is built up by directly extrapolating from all sub-systems assessed by means of the Calphad method. Then, the pseudo-binary sections that may provide the theoretical support for developing medium weight high entropy alloys will be calculated and examined by a series of experimental studies..

CFD-simulation of Siphone for Primary Aluminum Production: *Mohsen Amerisiahooei*[1]; [1]Almahdi-South Hormoz Aluminium

the tapping operation was carried out in the normal way.Today mathematical tools are used in the further development and optimisation of crocyble. CFD (computational fluid dynamics)simulation is a tool which has been successfully established in manydiverse sectors of industry. It is the intention of this article to present the simulation of a siphone which has been done using the commercial software FLUENT. Numerical simulation shall provide the plant constructor with information on the guiding of flows, temperature distribution, heat input and heat losses in a siphone.

Combinatorial Alloy Fabrication and Synergies with Predictive Frameworks for High-entropy Alloy Design and Down-selection: *Marcus Parry*[1]; Danielle Beatty[1]; Seongtae Kwon[2]; Taylor Sparks[1]; Jeffery Aguiar[2]; [1]University of Utah; [2]Idaho National Laboratory

High-entropy alloys (HEAs) are an emerging class of materials consisting of multiple principal elements. Due to entropic effects, HEAs are highly stable at elevated temperature with promising hardness, tensile strength, and corrosion resistance for potential structural applications in extreme environments. Due to the infinite compositional range of HEAs, discovery efforts benefit from a multifaceted experimental and computational approach. In this work, over 100 different alloys are synthesized focusing on near-equimolar compositions of the main constituent elements Fe, Cr, Ni, Mn, Al, Si, and Cu. The effects of alloying are investigated and reported in detail; specifically, microstructural and mechanical property characterization are achieved using X-ray/neutron diffraction, X-ray tomography, electron microscopy, hardness testing, tensile testing, and thermal analyses. Results are compiled to inform and validate modeling efforts, to increase data availability, and for use in the development of a statistically driven approach to differentiate compositions of interest during alloy design and testing.

Comparative Study of Efficiency of Methods of Gold Extraction from Anthropogenic Flotation Tails: Aigul Koizhanova[1]; Bagdaulet Kenzhaliyev[1]; *David Magomedov*[1]; Emil Kamalov[1]; Maria Erdenova[1]; [1]JSC «Institute of Metallurgy and Ore Benefication»

This paper shows the results of the comparative study of efficiency of methods of gold extraction from anthropogenic flotation tails by agitation cyanidation and biooxidation with following leaching. A representative sample was taken of flotation tailings at the gold extraction plant of AltyntauKokshetau. It was established that in the test sample contains 0.32 g/t Au and 0.62 g/t Ag.The extraction degree of gold from flotation tailings with 80% content of 0.071 mm fraction was 50%, and that with 90% content of 0.071 mm fraction was 60%. The extraction degree of gold from flotation tailings with 90% content of 0.044mm fraction at a solid-liquid ratio of 1:4 and a cyanide concentration of 1 g/dm3 is 65.2%. When using an active strain of thionic cultures the gold extraction degree was E Au= 72.1%.

Computational Discovery of Stable MXenes Alloy Phases: Xiao Xu Wang[1]; *Jun Jiang*[2]; Caiqun Wang[2]; Xu Cui[2]; Liutao Zhao[2]; [1]Beijing Computing Center, University of Science and Technology Beijing; [2]Beijing Computing Center

MXenes are a class of transition metal carbides and nitrides among the latest additions to the 2D world. Due to the excellent mechanical properties, metallic conductivity, and hydrophilic surface, MXenes are widely studied as electrodes in batteries and super-capacitors. MXenes alloys with more than one Metal element may allow incorporation of elements beside those included which, in turn, would enable addition of new properties and benefits for the property tuning. Here, we extend the use of modern high-throughput screening techniques with first principles calculations to screen all the entire $M_{n+1}X_n$(n=1–3) phase families for the thermodynamic stability. To complete the nontrivial task of selecting the most stable competing phases for these compositions, we systematically survey the Materials Project database. Our predictions provide guidance to experimental efforts for the synthesis of different MXenes alloy compounds.

Corrosion Resistance Improvement of Weathering Steel by Chemical Composition Optimization Using Support Vector Regression: *Luchun Yan*[1]; Kewei Gao[1]; [1]University of Science and Technology Beijing

The support vector regression (SVR) approach is proposed to establish a model for prediction of the atmospheric corrosion rate of weathering steel under different environment factors and alloy compositions. The predictive accuracy and generalization of SVR model were validated by applying independent test samples. The optimized SVR model was used as a simulator to predict the corrosion rate of weathering steel with specific alloy composition. Based on the simulation results, chemical composition of weathering steel with higher corrosion resistance was determined by using different machine learning algorithms. The selected samples were produced and its performance were evaluated through wet-dry cyclic corrosion test. These suggest that simulating model may be an effective methodology to develop weathering steel with high corrosion resistance.

Design of High Entropy Carbides Using Entropy and Enthalpy Descriptors: *Ruizhi Zhang*[1]; Mike Reece[1]; [1]Queen Mary University of London

High entropy carbides (HECs) are attracting considerable interest because of their promising applications as ultra-high-temperature ceramics. Design of HECs involves searching in a high-dimension multi-element chemical space for thermodynamically stable phases, which is formidable due to the vast searching space. Here we show that entropy and enthalpy descriptors from first principles calculations can be used to identify synthesizable compositions of HECs, where the descriptors are calculated using the standard error and the mean value of the energy distribution spectrum. Based on the calculations, we propose nine compositions of eight-cation HECs with high entropy and low enthalpy, and the cations' contribution to entropy and enthalpy is analyzed in detail. The effect of carbon vacancies on HECs is also calculated and discussed, as carbon off-stoichiometries are common in these carbides.

Design of Materials for Chemical Mechanical Planarization of Semiconductor Wafers: *Nagaravi Nadimpalli*[1]; Kshitij Saxena[1]; Rajdip Bandyopadhyaya[2]; Venkataramana Runkana[1]; [1]Tata Consultancy Services Ltd., Tata Research Development & Design Centre, Pune; [2]IIT Bombay

The chemical mechanical planarization (CMP) is one of the challenging and critical process steps in semiconductor fabrication. The stringent particle property requirements (particle size <100 nm, narrow particle size distribution (PSD), spherical morphology and crystalline structure) poses great challenges in the design and development of CMP products. The main objective of current work is to design and produce nanoparticle-based CMP slurries that meet the specifications of semiconductor wafer fabrication. We have developed a modeling framework by combining thermodynamics, reaction kinetics, computational fluid dynamics, and particle population balances to determine the CMP slurry PSD. The model was tested with published and in-house experimental data. We have then employed the modeling framework to design and develop CMP slurries with required specifications and produced them using lab-scale hydrothermal reactor.

Determination of the Phase Equilibria and Phase Transformations of Ti-Al-Nb System at Intermediate Temperatures Using Five Diffusion-components Couples Method: *Shuai Xu*[1]; Jianping He[1]; Klaus-Dieter Liss[2]; Junpin Lin[1]; [1]University of Science and Technology Beijing; [2]Guangdong Technion-Israel Institute of Technology

The Ti-Al-Nb ternary system includes three classes of alloys with great potential for application at intermediate temperatures, which are γ-TiAl alloys, O-Ti2AlNb alloys and σ+γ dual-phase alloys. Until today, the phase equilibria and phase transformations at intermediate temperautes have not been clarified. A diffusion couple named 'five diffusion-components couples' was designed in the present work. The 900 °C, 980 °C and 1010 °C isothermal sections were identified by comprehensively charactering the five diffusion-components couples using SEM, EPMA, EBSD, FIB, T-EBSD and TEM approaches. In-situ neutron diffraction approach and quenched alloys were used to verify the five diffusion-components couples results. Ten phases and eight phase transformations were identified in this ternary system at intermediate temperatures. Based on the results, the five diffusion-components couples are suitable for investigating the phase diagrams of the Ti-Al-Nb ternary system, which can solve the difficulties during studying the phase diagrams at half of the melting temperatures.

Development of Aeroengine Components through Multiscale Modelling: a Rao[1]; Ramakrishnan Raghavan[1]; Sankarasubramanian Ramachandran[1]; Balamuralikrishnan Ramalingam[1]; [1]Defence Metallurgical Research Laboratory
The hot-end components in gas turbine aeroengines are critical to the performance and safety of military aircraft, due to extremely random and severe loading patterns. Nickel-base superalloys, castings and forgings, are highly creep and fatigue resistant under such hostile high-temperature operating environments. Modelling was performed at multiple length-scales to determine the microstructural evolution in these alloys, together with continuum-level computations of material behaviour under processing and service conditions at component-level. *ThermoCalc* computations determined dendritic-level segregation, alloying elements' partitioning between the γ-matrix and γ'-precipitate phases, and alloy's susceptibility for topologically close-packed-phase formation. *Monte-Carlo* simulations for partitioning of alloying elements between γ-γ' phases, *Molecular-Dynamics* for Ni-Al solidification-kinetics induced anisotropy studies, and *Phase-fiend* simulations for γ-precipitates'evolution were carried out. *Dynamic Materials Modelling* and *Finite Element Analyses* facilitated engineering component development at the continuum-level. The results and challenges in integrating the techniques are discussed, apart from an ICME-based vision for component design.

Development of New Rare Earth Superalloy for Additive Manufacturing: *Maodong Kang*[1]; Jun Wang[1]; Haiyan Gao[1]; Baode Sun[1]; [1]Shanghai Jiao Tong University
The existing superalloys are difficult to meet the forming requirement of additive manufacturing. In this study, Ni-Al alloy was select as the Matrix Material. Base on the phase diagram calculation, Several Rare Earth Elements were selected as candidates to design new superalloy. The new superalloys have higher heat resistance temperature. After preparation of Button Samples by Vacuum Non-consumable Arc Furnace Melting, high-throughput Laser ablation method was used to evaluate the formability properties of additive manufacturing. Preliminary results shows that the different Rare Earth element addition present different crack phenomenon,such as the density, width and length of cracks. The crack formation tendency is closely related to laser processing parameters. In addition, surface roughness also shows great differences. However, the new superalloy is more brittle than traditional Superalloys. More work should be carried out to improve the plasticity of new Rare Earth Superalloy.

Development of Prediction Techniques for Long-term Performance of Mg Alloys Based on Materials Integration Approach: *Daisuke Egusa*[1]; [1]University of Tokyo
Mg alloys have been gathering wide attentions as an application to structural materials owing to their high strength/weight ratio. For practical use, prediction and control of material performance over a long period of time such as fatigue and corrosion are required, but basic knowledge for predicting long-term performance in Mg alloys is still insufficient. In recent years, as a means to solve the difficulties in such development, a material designing method "Materials Integration" integrating various technologies such as computational material science and data science has developed. We have been developing a system for efficiently predicting long-term performance of Mg alloys, adapting Materials Integration approach. In the present study, we focus on developments of prediction techniques of mechanical properties based on database that contains process and microstructural information of materials.

Development of Time-temperature-transformation and Properties Diagrams for Alloy 282 Using a Novel Arc Heat Treatment Technique: *Ceena Joseph*[1]; Kevin Vattappara[2]; Vahid Hosseini[3]; Kjell Hurtig[3]; Joel Andersson[3]; [1]GKN aerospace.com; [2]KTH university; [3]University Väst
Alloy 282 is γ'-strengthening alloy with excellent combination of high temperature properties and fabricability. As it is relatively new alloy, the developing time-temperature-transformation diagram plays crucial role in understanding transformation of different phases in this alloy with different temperatures and times. A newly developed heat treatment technique, called arc heat treatment, will be employed to heat treat the samples where a steady state melt pool forms a few seconds after arc applied and constant temperature isotherms forms next to the weld pool. This results in a unique graded microstructure within the whole range of temperatures from melting point to room temperature. This approach decreases the total number of samples compared to other techniques, as all temperatures are present in one sample. Different times will be applied to investigate the evolution of microstructure and hardness at various time and thermodynamic calculations will be performed to compare the results with equilibrium condition.

Development of Workflow Subsystems and Structural Material Database with Direct Handling of Materials Parameters: *Kaita Ito*[1]; Satoshi Minamoto[1]; Takuya Kadohira[1]; Makoto Watanabe[2]; Masahiko Demura[1]; Manabu Enoki[3]; [1]Integration G, National Institute for Materials Science; [2]SIP-MI Laboratory, National Institute for Materials Science; [3]Department of Materials Engineering, The University of Tokyo
A workflow designer and player were developed as core subsystems of the Materials Integration (MI) system. A major feature of these workflow subsystems is direct handling of material parameters as inputs and outputs of the modules in workflow. Unlike typical workflow systems, they do not rely on files and data of a specific application software. By defining inputs and outputs in this way, direct information on the accuracy and effective input range of each prediction model can be accumulated. In order to respond closely to the MI workflow subsystems, a novel design structural material database was also developing. In this database, material is defined as an accumulation of manufacturing processes. Also, experimental data can be attached to each step of processes.

Effect of Layer Thickness on the Residual Stresses of CIGS Solar Cells due to Hotspot: *Hansung Kim*[1]; Da Xu[1]; [1]Purdue University Northwest
In this paper, we investigated the effect of layer thickness on the residual stresses of copper indium gallium diselenide (CIGS) solar cells caused by cooling to room temperature from hotspot temperatures of 200°C, 300°C, 400 °C using Finite Element Method (FEM). Our simulated CIGS is composed of four layers: ZnO, CdS, CIGS, and Mo. We were able to quantify the effect of each layer thickness on the average stresses of each layer for different temperatures. It was found that Mo/CIGS interface goes through the stress type transition from compression to tension while CIGS/CdS interface goes through stress type transition from tension to compression for all hotspot temperatures. However, the CdS/ZnO interface does not go through stress type transition since both layers have compressive stress for all hotspot temperatures. However, the ZnO layer has a higher compressive stress than that of CdS layer.

Effect of Temperature on the Mechanical Properties of Hydrogel: Modeling and Experiment: *Hansung Kim*[1]; Da Xu[2]; Aditya Lingaraju[1]; Herve Kpoffon[1]; Harvey Abramowitz[2]; [1]Purdue University Calumet; [2]Purdue University Northwest
Hydrogel is getting significant attention as a biomedical material in the applications of tissue engineering and drug delivery. Since a hydrogel is a network of polymers containing significant amount of fluid, it shows a viscoelastic behavior and it's mechanical properties are influenced by temperature. We investigated the effect of temperature (T) on the Young's modulus (E) of a commercial hydrogel using Atomic Force Microscopy (AFM). Hertz contact theory was used to calculate the young's modulus of Hydrogel based on AFM force-displacement curves at different temperatures ranging from 20°C to 50°C. Activation energy of Young's modulus of hydrogel was obtained through Arrhenius equation. Linear relationship between ln(E) and (1/T) confirm that Hydrogel Young's modulus follows the Arrhenius equation. Moreover, we were able to model viscoelastic behavior of the hydrogel using finite element method (FEM) analysis. Our FEM simulation results of force-displacement curves show a good agreement with AFM experimental data.

Elastic Anisotropy and Mechanical Property of Au-Sn Intermetallics from First-principles Calculations: Kai Xiong[1]; *Yong Mao*[1]; [1]Yunnan University
Au-Sn solder is extensively employed in the electronic packaging of optoelectronic and high-powered electronic components due to its superior mechanical and thermal conduction properties. However, there are a large number of brittle intermetallic phases in Au-Sn alloy. In this work, the structural, mechanical, electronic and thermodynamic properties of the four typical Au5Sn, AuSn, AuSn2, and AuSn4 intermetallics are systematically invesitgated by the first-principles calculations based on density functional theory (DFT) to provide useful data for further investigating and designing new Au-Sn solder materials.

Electronic Transport in Multi-component Amorphous Semiconductors: *Juhi Srivastava*[1]; Suhas Nahas[1]; Somnath Bhowmick[1]; Anshu Gaur[1]; [1]Indian Institute of Technology Kanpur

Multi-cation based amorphous oxide semiconductors (AOS) and specifically a-IGZO is the most researched material which has reached commercialization with mobilities exceeding 15cm2/V-s for backplane TFT applications. Recently a multi-anion based amorphous semiconductor, a-ZnON is shown to achieve Hall mobilities an order of magnitude higher compared to multi-cation based AOS. In order to understand the nature of electronic conduction in these amorphous semiconductors and how they are differentiated, first principle electronic structure calculations are performed to study their electronic transport properties. As proposed in literature, electronic conduction in these ionic semiconductors is through overlapping s-orbitals of metal-cation pairs. With the structural analysis of these amorphous phases, overlap between different metal-cation pairs has been quantified. The ease of electronic transport (electron-mobility) is found to be correlated to the extent of orbital-overlap. By calculating the pair-wise orbital-overlap integrals, we have tried to predict the most-probable electronic conduction path in multi-component amorphous semiconductors.

Exploring Correlations between Properties Using Artificial Neural Networks: *Yiming Zhang*[1]; Shoufeng Yang[2]; Julian Evans[3]; [1]Ningbo Institute of Industrial Technology, Chinese Academy of Sciences; [2]KU Leuven; [3]University College London

The traditional aim of materials science is to establish the causal relationships between composition, processing, structure and properties with the intention that eventually, these relationships will make it possible to design materials to meet specifications. This paper explores another methodology. There are relationships between properties that can be discerned and used to make predictions so that knowledge of some properties in a compositional field can be used to predict others. We use the physical properties of the elements as a data set because it is expected to be both extensive and reliable and we explore this methodology by showing how it can be applied to predict the polarizability of the elements from other properties.

First-principles Investigation on the Stability and Oxygen Adsorption Behavior of a Ti2AlNb/TiAl Interface: *Yue Li*[1]; Jianhong Dai[1]; Yan Song[1]; [1]Harbin Institute of Technology at Weihai

The stability of a interface between O-phase Ti2AlNb (1 -1 0) surface and B2-phase TiAl (2 1 -1) surface was studied by first principles calculations to investigate the atomic matching behavior. A coherent twin boundary with extremely small misfit degree was found, The calculated formation energy and the electronic structure illustrate that the interaction is strong. The adsorption of a single oxygen atom at the interface was estimated thermally stable by adsorption energy. The present research indicates the existence of O/B2 interface may lead to influences on the oxidation resistance of Ti2AlNb alloys.

Gleeble and LUMet (Laser Ultrasonic Metallurgy): *Michael Hudack*[1]; [1]Dynamic Systems Inc

In the metals industries and materials research groups the Dynamic Systems Inc (DSI) Gleeble systems are used in industry and Academia to optimize welding, casting, forging, and rolling processes to improve processes for new or existing materials in the laboratory while keeping production facilities producing with minimum downtime via small samples producing invaluable processing maps via 10,000C degrees/second and up to 20 tons compression during live, real-time, in-situ physical simulation processes. Gleeble and the LUMet model complement and further document mathematical computational formulae for material characterization. LUMet (Laser Ultrasonic Metallurgy) as an option monitors microstructures at high-temperatures on a Gleeble 3500 or 3800 to study: recrystallization; grain growth; grain size; phase transformations; elastic constants; and texture within Gleeble at the same force of 20 tons at 10,000C degrees/second. LUMet makes its unique measurements by generating and detecting ultrasound pulses in a sample with lasers up to 50 measurements per second.

Hall-Petch Relation and Boundary Strengthening in Mg Alloys: *Mohsen Taheri Andani*[1]; Aaditya Lakshmanan[1]; Mohammadreza Yaghoobi[1]; Veera Sundararaghavan[1]; John Allison[1]; Amit Misra[1]; [1]University of Michigan

Understanding the strengthening mechanisms of individual grain boundaries is key to assess the mechanical properties of polycrystalline materials. Hall-Petch relationship is a well-known equation which expresses such effects by predicting the yield strength of materials as a function of average grain size. In spite of the extensive research conducted to understand this relationship, many fundamental questions remain unanswered. The objective of this work is to utilize a novel cross-correlation-based EBSD experiment to assess the stress variation near the interaction of a slip band with a grain boundary in Mg alloys. The calculated stress concentration induced can be fitted with a developed theoretical model, from which micro-Hall–Petch coeffcients for different grain boundaries can be deduced. Obtaining such unprecedented microstructural measurements will help to accurately calibrate the crystal plasticity finite element framework model to predict the mechanical response of magnesium alloys, considering the grain size and geometrical features of grain boundaries.

Heuristics for the Design of New Materials: *Graham Schaffer*[1]; [1]University of Melbourne

The design of new materials is similar to the design of both other engineered artifacts and to the evolution of new technologies, but the process of materials design itself is seldom studied. This study examines best practice in materials design with the aim of constructing a theory of materials design and developing a materials design heuristic that limits the search for solutions in large search spaces, such as multidimensional materials property space. A multiple case study approach is employed, using expert interviews to capture the stories behind effective materials development programs and provide insight into tacit expert knowledge in order to construct systematic procedural knowledge. Participants are research scientists and engineers at universities, institutes and companies with extensive materials design and development experience. Preliminary results suggest that materials evolve into the adjacent possible through many ideation-prototyping-evaluation cycles, enhanced by computational modelling, the integration of disparate knowledge sets and competitive co-creation.

ICME Design for Lightweight Steels: Thermodynamics, Diffusion Mobility, Volume and Yield Strength Predictions: *Weisen Zheng*[1]; Huahai Mao[2]; Yanlin He[1]; Malin Selleby[2]; John Ågren[2]; Ping Yan[3]; Qiang Zeng[3]; Xiao-Gang Lu[1]; [1]Shanghai University; [2]KTH Royal Institute of Technology; [3]Central Iron & Steel Research Institute

In the austenitic lightweight steel, the nano-precipitation of the K-carbide within the austenitic matrix significantly contributes to the improvement of the yield strength. In the present work, the yield strength was predicted within the framework of the ICME approach. The thermodynamic, diffusion mobility and volume databases for lightweight steels were constructed using both computational and experimental techniques, including CALPHAD, ab initio calculations and diffusion-couple method. Based on the present databases, the precipitation of the K-carbide during aging was simulated to obtain the volume fraction and mean particle radius. Combining with the models for the solid solution strengthening, grain boundary strengthening, coherency strengthening, anti-phase boundary strengthening and modulus strengthening, the yield strength is predicted for the austenitic lightweight steel with finely dispersed nanometre-sized K-carbide. The quantitative relationship between the alloy composition, aging parameters, precipitation behavior and the yield strength was established for lightweight steels in the present work.

Image Based Analysis for Stress Environment in Duplex Structure Stainless Steels: Carley Ann Suarez[1]; Sanjay Sarma Oruganti[1]; Yong Yang[2]; Appajosula Rao[3]; *Ramana Pidaparti*[1]; [1]University of Georgia; [2]University of Florida; [3]Nuclear Regulatory Commision

The cast austenitic stainless steels (CASS) are highly corrosion-resistant Fe-Cr-Ni alloys with austenite (γ)-ferrite (δ) duplex structure or polycrystalline austenite structure, depending on their chemical compositions and processing routes. The attractive combination of properties resulted from duplex phase structure allows their wide applications in many industries. Using the experimental data of SEM micrographs of the nanostructure CASS test sample, finite element (FE) analysis models were developed to investigate the mechanical stress environment under uniform pressure and strain loading conditions. The results of maximum von-Mises stresses and maximum shear strain at ferrite phases are about 18%-24% higher, and about 4%-7% less under uniform strain loading in comparison to uniform pressure loading. Using these stress/strain values and based on material fracture stress, possible crack initiation locations can be identified. Currently, more results are being obtained and the sensitivity analysis to material property is investigated and results will be presented at the conference.

Interaction between Cu and Cr Coadsorption on MnS Inclusions in Low Alloy Steel and Study of the Interfaces between a-Fe and MnS: *Wenting Lv*[1]; Luchun Yan[1]; Xiaolu Pang[1]; Huisheng Yang[1]; Lijie Qiao[1]; Yanjing Su[1]; Kewei Gao[1]; [1]University of Science and Technology Beijing
The first principles calculations based on density functional theory and TEM experiments were employed to investigate the coadsorption of Cu and Cr on MnS inclusions in low alloy steel and the interfaces between a-Fe and MnS. The enrichments of Cu and Cr on MnS inclusions were observed by TEM. The atomic structures, electronic and energetic properties of clean and Cu or Cr adsorbed MnS surface were calculated. Besides, the interfacial properties such as the work of adhesion (Wad), interface energy (γint) and electronic structures of the interfacial structures were also calculated. Results show that Cu and Cr promote the adsorption of each other on MnS (100) surface and Fe (110)/MnS (110) is the most stable interfacial structure among the nine candidate interfaces. The orientation relationship of α-Fe and MnS was identified as Fe (110) // MnS (110) by TEM, which is in good accordance with the calculated results.

Interface Strengthening Mechanisms of Ti/CFRP Fiber Metal Laminate after Adding MWCNTs to Resin Matrix: *Hao Wang*[1]; Kai Jin[1]; Jie Tao[1]; [1]Nanjing University of Aeronautics and Astronautics
Since the Metal/resin interface delamination is the biggest challenge for fiber metal laminate (FML) applications, there is an urgent need to strengthen the metal/resin interface. In this study, multi-walled carbon nanotubes (MWCNTs) were added to a polyimide (PI) matrix to improve the interfacial strength of titanium/polyimide (Ti / PI). Metal-inorganic-organic systems and related equations were developed to describe interface behavior. The effect and mechanism of the system on MWCNTs were analyzed by molecular dynamics (MD) simulation. The analytical results are consistent with the shear test. It was found that MWCNTs can significantly improve interface properties through van der Waals forces and chemical bonds. If the MWCNT is perpendicular or at 45° to the Ti surface, the interface strength will reach a maximum. The methods proposed by MD simulation and experiments can also be used to study graphene or other strengthening phases.

Interfacial Dielectric Analysis in Polymer Nanodielectrics from First Principles: *Yumeng Li*[1]; Xin Chen[1]; [1]University of Illinois Urbana Champaign
High permittivity polymer-based nanocomposites attract a lot of attentions due to their potential applications as high energy density storage devices with the advantage of light weight and easy processing. While the effective dielectric properties of the nanocomposites are greatly affected by the individual properties of nanofillers and polymer matrix, the interface and interphase regions between the nanofillers and the matrix is believed to play a critical role on the bulk properties of the nanocomposites. In this paper, we will understand the fundamental mechanisms governing the local dielectric properites in the interfacial regions of the graphen/ polyvinylidene difluoride (PVDF) dielectric nanocomposites, thereby establishing the structure-property relationship to assist the rational design of nanodielectrics.

Investigating the Role of Impurities in Grain Boundary Phase Transformation with Atomistic Simulations: *Shengfeng Yang*[1]; [1]Indiana University; Purdue University Indianapolis
Impurities segregated at grain boundaries (GBs) can cause transformation of GB phases in various materials. GB phase transformation can affect a broad range of materials properties such as strength and ductility. We use atomistic simulations to predict structures of equilibrium GB phases and the transformation between them at finite temperatures. Two examples, S-doped Ni and Ni-doped Mo, will be discussed. The formation of bilayer phase and amorphous phase in S-doped Ni is observed from simulations and validated by experiments. The effect of transition between these two phases on GB embrittlement are studied. In the example of Ni-doped Mo, a first-order GB phase transition from clean phase to bilayer phase is identified and validated by DFT calculations. The simulation results are used to construct GB "phase" diagram, which is a useful tool to reveal the GB excess of dopants and structural disorder as functions of the bulk concentration and temperature.

Investigation of Stiffness Coefficients of Pristine Graphene at Various Scales: *Chaitanya Sagar*[1]; Arun Rony[1]; Viswanath Chinthapenta[1]; [1]Indian Institute of Technology, Hyderabad
The mechanical properties of pristine Graphene are calculated at electronic-, atomistic- and continuum scale. At the electronic scale, DFT simulations are carried out at the ground state (T=0) using quantum espresso (QE), elastic stiffness and interatomic potentials are obtained from the analysis. The atomistic scale simulation are performed using LAMMPS. The interatomic potential needed is supplied from the electronic scale simulations using the MEAM potential calibration tool. Further, in the continuum scale, FEM calculations are carried out by modeling bond as a continuum beam element. The stiffness parameters are calibrated for pristine graphene with the backing of atomistic and electronic scale simulations. The obtained stiffness coefficients from various scales are compared.

Investigation on Phase Transformations in Inconel 718 Alloys Manufactured by Suction Casting and Additive Manufacturing: *Yunhao Zhao*[1]; Wei Xiong[1]; [1]University of Pittsburgh
Continuous cooling processes can affect phase transformation kinetics and are hence critical in post-processing of Inconel 718 Ni-base superalloy. In this work, Inconel 718 alloys are prepared by suction casting and powder-bed laser melting, subjected to homogenization with different durations and cooled at different rates. Electron microscopic characterization and quenching dilatometric analysis show the Delta phase as the main precipitate during cooling and the precipitation kinetics is influenced by homogenization. Qualitative analysis indicates different Nb-segregation intensities are caused by variation of homogenization, which further influences the precipitation kinetics of the Delta phase. Continuous cooling transformations are simulated using the Thermo-Calc software package with experimental calibration/verification. The interfacial energies of precipitates are determined from the simulation and found to be able to support the analysis by Johnson-Mehl-Avrami-Kolmogorov model. The present study on phase transformations is beneficial to the optimization of post-processing in advanced manufacturing for Inconel 718 alloys.

Knowledge Graph: A New Way from Materials Database to Knowledge Base: *Quan Qian*[1]; Yuexing Han[1]; [1]Shanghai University
As we all know, materials database is playing a very important role in current data-driven based new materials design and development. However, traditional relational database, although can store data in 2-dimensional data format, it has heavy limitations on representing these complex relations among different types of data. Therefore, how to save and utilize materials data, especially the complicated data relations, is almost the core and difficult questions in data-driven based materials research. In this talk, I will focus on a quite different topic that how to save and represent the data relations by utilizing the new technology: knowledge graph. And for a specific alloy example, I will give some details of how to build a materials knowledge graph? What are the typical applications of knowledge graph, such as graph searching, classification, question-answer system, and graph reasoning? And in addition, what is the roadmap from database to knowledge base?

Machine Learning Assisted Composition Design of Copper-base Alloys with High Strength and High Electrical Conductivity: *Huadong Fu*[1]; Hongtao Zhang[1]; Jianxin Xie[1]; [1]University of Science and Tehcnology Beijing
Even 0.1wt% change of alloying element content will have a great impact on properties in copper alloys and clarifying the influence of the composition on the properties of the alloy has important guiding significance for the rational design of the composition. In order to break through the limitation of alloy elements in the samples, and design the high-strength and high-electrical-conductivity copper alloy composition efficiently, the main descriptors for the tensile strength and electrical conductivity of the alloy were screened by machine learning method respectively. Then the suitable strengthening alloy elements were selected in the periodic table depending on the variation law of properties with descriptors. With the main descriptors as input, the tensile strength model with accuracy greater than 98% and the electrical conductivity model with accuracy greater than 93% were established by using the support vector machine algorithm, and copper alloys with better properties were designed.

Machine Learning Prediction of Uranium-based High Entropy Alloys with High Strength: *He Huang*[1]; [1]China Academy of Engineering Physics
Uranium-based high entropy alloys can be used as an important candidate for fission fuels in future. Several uranium-based solid solution alloys with bcc structure were successfully predicted by machine learning and verified by experiments. The calculation results show, the characteristic variable which influences the formation of solid solution phase is mostly from electronic structure. The compressed yield strength of the alloy with double bcc structures is about 1.2 GPa and higher than that of other two alloys with single bcc structure. The reason for differences of compression property among these alloys is further analyzed by various characterizations.

Materials Data Specification: Methods and Use Cases: *Quan Qian*[1]; Yuexing Han[1]; [1]Shanghai University

With the extremely fast development of Materials Genome Initiative (MGI) and Materials Informatics (MI), expressing materials data formally, semantically and scientifically is urgently demanded. According to the features of materials data, we proposed a hierarchical representation of materials data specification described by Backus-Naur Form (BNF), and then use XML Schema Definitions (XSD) to implement the BNF. Subsequently, detailed XSD writing guidelines for simple key-value materials data, tabular structure data and unstructured data are given. Moreover, in this paper, we provide the real programming sourcecode to validate materials data in XML format with predefined XSD template. Finally, as use cases, the general specifications for computational data and experimental data are presented for researchers reference.

Mathematical Modeling and Optimization of Polymer Composite Pine Fins: *Yaser Rihan*[1]; [1]Egypt

Heat sinks, composed of arrays of variously-shaped fins are used for the thermal packaging of most categories of electronic equipment. Optimum design must involve the least-mass and least-energy consumption of heat sinks and include both geometric and material selection considerations. The high thermal conductivity polymer-fiber composites using carbon fiber and graphite fillers to increase the thermal conductivity offer a most promising alternative to conventional heat sink materials such as aluminum and copper. To achieve the goals of sustainable development, the design and use of such heat sinks involves a subtle balance between a superior thermal design, minimum material consumption, and minimum pumping power. The present paper appears to provide a systematic study of the thermal performance of an air-cooled heat sink fabricated of a relatively high thermal conductivity PPS polymer. A staggered pin fin array has been used for the design and optimization of such air-cooled, natural convection heat sink.

Microstructural Evolution during Intercritical Annealing of Medium-manganese Steels: *Josh Mueller*[1]; Emmanuel De Moor[1]; John Speer[1]; David Matlock[1]; Kyoo Sil Choi[2]; Xiaohua Hu[3]; Xin Sun[3]; [1]Colorado School of Mines; [2]Pacific Northwest National Laboratory; [3]Oak Ridge National Laboratory

Intercritically annealed medium-manganese (Mn) steels have microstructures containing carbon (C) and Mn enriched austenite that forms during intercritical annealing. A wide range of mechanical properties are achievable which are dependent on the austenite content and composition. By predicting the microstructural development during intercritical annealing, phase field simulations can aid in the development of medium-Mn steel grades to target specific strength-ductility combinations. However, the parameters and mechanisms that are significant for intercritical annealing are not fully understood. Phase field simulations for the microstructural evolution of medium-Mn steels can contain many parameters including those pertinent to, austenite nucleation, ferrite recrystallization, solute transport, interface mobility, and texture. The work discussed will show phase field simulations using a commercial software package, MICRESS®, and how varying some or combinations of parameters can affect simulation results such as austenite composition, content, and growth rate. Comparison to experimentally intercritically annealed medium-Mn steels will also be shown.

Microstructure Sensitive Critical Plastic Strain Energy Density Criterion for Fatigue Life Prediction across Various Loading Regimes: *Ritwik Bandyopadhyay*[1]; Veerappan Prithivirajan[1]; Alonso Peralta[2]; Michael Sangid[1]; [1]Purdue University; [2]Honeywell Aerospace

The plastic strain energy density (PSED) is considered as a metric for fatigue life prediction. Crystal plasticity finite element simulations are used to compute the microstructure-sensitive PSED within a Nickel-based superalloy. Bayesian inference method is utilized to calibrate the critical PSED. Subsequently, the calibrated value is used to predict fatigue lives at nine strain ranges including R-ratios of 0.05 and -1 using nine statistically equivalent microstructures (SEMs). For each strain range, the predicted lives from all SEMs are found to follow a log-normal distribution. For a given R-ratio, the scatter in the predictions is observed to be increasing with decreasing strain amplitude and is indicative of experimental observations. Finally, the log-normal mean lives at each strain range are observed to be in good agreement with experimental data. Since a constant critical PSED value predicts fatigue lives reasonably well at various loading regimes, it is hypothesized to be a material property.

Modeling of Gas Bubble Evolution in Nuclear Fuel under Temperature Gradient and Pitting Corrosion in Metals with Passivation: *San-Qiang Shi*[1]; [1]Hong Kong Polytechnic University

In the first part of the talk, a quantitative phase-field model was developed to predict the evolution of gas bubbles in nuclear fuel under temperature gradient. The model takes into account temperature, gas bubble internal pressure, interfacial energy between bubble and matrix, and elastic strain energy within the material. The model can handle realistic equilibrium concentrations of vacancies and gas atoms. Case studies include time-dependent bubble size evolution as a function of temperature, vacancy and gas generation rates; interaction between gas bubbles and distribution of gas bubble sizes, etc. In the second part of the talk, a multi-phase-field model for pitting corrosion in metals with passivation will be presented. The mass transport in the electrolyte, electrochemical reactions in the electrolyte/electrode interface, and insoluble corrosion product are taken into consideration in the model in order to simulate metal corrosion in a corrosive environment with passivation.

Modeling of Temperature-dependent Impact Properties of 3D Printed 15-5 Stainless Steel: Sugrim Sagar[1]; Yi Zhang[1]; Jian Zhang[1]; Yeon-Gil Jung[2]; *Jing Zhang*[1]; [1]Indiana University-Purdue University Indianapolis; [2]Changwon National University

3D printed 15-5 stainless steel specimens were fabricated using the powder bed fusion (PBF) process. The impact properties of the 3D printed 15-5 stainless steel at low temperature (77 K), room temperature (298 K) and high temperature (723 K) were investigated using the Charpy impact test. In parallel to the experiments, a Johnson-Cook phenomenological flow stress model along with damage parameters was implemented in LS-DYNA, and the impact energies were computed. The results of the experimental and numerical modeling were in a good agreement.

Module-design and Prediction of Nonlinear Optical Materials with High Performances: *Zhihua Yang*[1]; [1]Xinjiang Technial Institute of Physics and Chemistry

In the exploration of ultraviolet and deep ultraviolet nonlinear optical materials, compounds only containing tetrahedral units commonly have problems such as low second harmonic generation and a small birefringence. However, it is easier to form a three-dimensional network structure, which is favorable for large-size crystal growth. On this basis, we selected a series of dominant units such as (BO3F)4-, (BO2F2)3-, (BOF3)2-, and PO4 units with a zipper arrangement. By designing and assembling these dominant units, new materials with phase matching wavelengths reaching the deep ultraviolet area are designed. References 1] B. Lei, Z. Yang*, et.al., J. Am. Chem. Soc.2018, 140, 10726. 2] B. Zhang, Z. Yang*, et. al, Angew. Chem. Int. Ed. 2017, 56, 3916. 3] B. Lei, Z. Yang*, et. al, Chem. Commun. 2017, 53, 2818.4] B. Zhang, Z. Yang*, et al, Chem. Mater., 2018, 30,5397.

Multi-scale Simulation of the Deformation and Transformation Behavior in Titanium Alloys: *Dongsheng Xu*[1]; Dejun Yu[1]; Xuexiong Li[1]; Jinhu Zhang[1]; Gang Zhou[1]; Hao Wang[1]; Rui Yang[1]; [1]Institute of Metal Research, Chinese Academy of Sciences

Multi-scale simulations of the deformation and phase transformation behavior in titanium based alloys under hot processing and service conditions are carried out. It was found that the deformation mechanisms in both titanium and titanium aluminide are sensitive to the deformation condition. External stress may have strong influence on the deformation microstructure and phase transformation, therefore affecting variant selection and texture formation. High throughput simulation were carried out to search for the alloying element that may promote the activation of certain deformation mechanisms such as twin in HCP titanium and pseudo-twin in TiAl. FEM simulation of the Gleeble compression test show that the constitutive relation obtained from Gleeble test may have substantial errors due to the non-uniform temperature and strain distribution in the sample. A correction scheme is proposed to obtain more accurate constitutive relations.

Multi-scaled Mapping Analysis of Cu-rich Phase in USC Heat-resistant Steel during Isothermal Aging: *Lixia Yang*[1]; Lei Zhao[1]; Xuejing Shen[1]; Zhengdong Liu[1]; Xiaojia Li[1]; Haizhou Wang[1]; [1]China Iron & Steel Research Institute

G115 is a novel heat-resistant steel used for 650 °C USC power plants. The high-temperature strength of G115 has been improved by adding 1 wt.% of Cu. However, there is not clear in the existing form, distribution and mechanism of Cu in G115. Herein, a multi-scaled mapping characterization method to select feature regions and units is developed and applied to the analysis of Cu-rich phase in G115. It is found that the Cu-rich phase with FCC structure has been formed. The Cu-rich phase is often symbiosis with M23C6 and Laves phase in the lath interface or grain boundary. As aging time prolongs, the content of Cu in the matrix decreases gradually, and Cu precipitates grow up. Our work provides an effective method for high-throughput screening of feature units (‘gene’) in G115, and would offer an efficient experimental tool for characterization and development of new materials.

Multiscale Modeling of Microstructural Evolution Induced by Thermomechanical Processing in Ti-6Al-4V Alloys: *Arun Baskaran*[1]; Sagar Bhatt[1]; Daniel Lewis[1]; Antoinette Maniatty[1]; [1]Rensselaer Polytechnic Institute

A collaborative effort combining Monte Carlo(MC) and Phase Field simulations, experimental results, and feedback control has been created to allow for enhanced manufacturing of Ti-6Al-4V at a lower cost. Ti-6Al-4V exists in two primary phases, the HCP α phase and the BCC β phase. The MC grain growth model is used to simulate prior-β grain growth, while a finite element crystal plasticity model is employed to model microstructural evolution induced by deformation and compute heterogeneous stored energy. A multi phase field formalism is adopted to model the nucleation and growth of all unique α-variants from a β matrix, by incorporating the crystallographic symmetry and the orientational relationship between the two phases. We report the work in progress towards augmenting our model with the microelasticity theory of Khachaturyan, in order to study the role of elastic strain field and other processing conditions in α-variant selection and consequently the morphology obtained. Reference: 1. Khachaturyan AG. Theory of structural transformations in solids. New York: John Wiley & Sons; 1983Acknowledgement: This research is sponsored through a grant from the National Science Foundation, Award CMMI-1729336, DMREF: Adaptive control of Microstructure from the Microscale to the Macroscale. The authors acknowledge our co-workers on this grant providing experimental, analysis and controls expertise, Professors Robert Hull and John Wen, graduate students Genevieve Kane, Anant Kekre, and Zhenhan Huang, and undergraduate student Michael Allahua

PanDiffusion: High-speed Multi-component Diffusion Simulation: *Duchao Lv*[1]; Shuanglin Chen[1]; Chuan Zhang[1]; Weisheng Cao[1]; Fan Zhang[1]; [1]CompuTherm LLC

CALPHAD-based simulation of diffusion problems, such as diffusion couple, homogenization, and particle dissolution, have been intensively used in alloy design. However, diffusion simulation in multi-component alloys is still challenging since it is prohibitively expensive computationally to calculate the required thermodynamic/kinetic quantities. To overcome the computational bottleneck, the PanDiffusion module of PandatTM software was developed and connects with PanDataNet, a thermodynamic data management system. Examples of multi-component diffusion couples display that PanDiffusion is revolutionizing kinetic simulation with a significant improvement of both reliability and efficiency. Diffusion simulation using PanDataNet is several orders of magnitude faster than the direct access to PanEngine, and calculated quantities are saved for future use. A rich variety of applications is displayed including homogenization, particle dissolution, and phase transform, and in several different geometries, thermal histories, and boundary conditions.

Phase Field Modeling of Dendritic Microstructure in Additively Manufactured Titanium Alloy: *Jing Zhang*[1]; Linmin Wu[1]; Lingbin Meng[1]; Jian Zhang[1]; [1]Indiana University-Purdue University Indianapolis

In this work, using Ti-6Al-4V as a model system, the phase field method is applied to simulate the microstructure evolution in additively manufactured metals. Frist, the fundamental governing equations are presented. Then the effects of various processing related parameters, including local temperature gradient, scan speed and cooling rate, on dendrites morphology and growth velocity are studied. The simulated results show that the dendritic arms grow along the direction of the heat flow. Higher temperature gradient, scan speed and cooling rate will result in small dendritic arm spacing and higher growth velocity. The simulated dendritic morphology and arm spacings are in good agreement with experimental data and theoretical predictions.

Poly (Vinyl Alcohol) (PVA) Meniscus Development Personalized with the Aid of Rapid Prototyping: *Celio Wataya*[1]; Cecilia Zavaglia[2]; [1]EEEM Maria Helena Valente Tavares; [2]State University of Campinas

The material selected for obtaining a prosthesis is poly (vinyl lcohol) (PVA), being a polymer of low production cost, and easy to obtain good characteristics for use as a biomaterial. The results of mechanical tests have confirmed the effectiveness of this material. Values like compression module 37.4 MPa (± 1.74), the modulus of creep indentation E = 3,6 MPa (± 0.6), tensile modulus and strain, respectively equal to s= 3.2 MPa (± 0.3) and ε = 148.4% (± 39) show the possibility of use of PVA as well as replacement ofthe meniscus human. Other tests were also conducted as in vitro and in vivo tribological and Differential Scanning Calorimetry (DSC), with results favorable to that end. To obtain the meniscus of PVA in the dimensions of the meniscus of the patient if the technology used rapid prototyping (RP)

Prediction of Microstructure of Interdendritic Eutectic Phase during Solidification of Multi-component Alloys: *Miaomiao Chen*[1]; Qiang Du[2]; Huadong Fu[1]; Biao Hu[3]; Yong Du[4]; Lian Zhou[1]; Jianxin Xie[1]; [1]Beijing Advanced Innovation Center for Materials Genome Engineering, Institute for Advanced Materials and Technology, University of Science and Technology Beijing; [2]SINTEF Materials and Chemistry; [3]School of Materials Science and Engineering, Anhui University of Science and Technology; [4]State Key Lab of Powder Metallurgy, Central South University

A multi-scale model is proposed to describe the interaction between long-range dendritic arm diffusion and diffusion between divorced eutectic particles. The model is applied to predict precipitation kinetic of interdendritic divorced eutectic phases during the solidification of Al-Mg-Si and Cu-Ni-Si alloys. Under the same total solute elements content, the effects of each element composition and cooling rate on the evolution of important microstructure features are predicted, including phase type and volume fraction, and size distribution of interdendritic eutectic phase. It is found that the ratio of solute elements content directly affects the type and volume fraction of final phases. And cooling rate affects the degree of back diffusion, which significantly affects the volume fraction of the eutectic phase. The simulation results of the multi-scale computational model agree well with the experimental results reported in the literature demonstrating the proposed model are valuable in guiding solidification microstructure engineering for multi-component alloys.

Recrystallization and Grain Growth Simulations for Multiple-pass Rolling and Annealing of U-10Mo: *William Frazier*[1]; Chao Wang[1]; Shenyang Hu[1]; Zhijie Xu[1]; Vineet Joshi[1]; [1]Pacific Northwest National Laboratory

A simulation model of recrystallization and grain growth has been developed to investigate grain structure evolution during deformation and heat treatment in polycrystalline UMo fuel. SEM images of microstructures were directly used as input for closed loop simulations of multiple rolling and annealing passes. FEM calculations of deformation and Potts Model simulations of recrystallization and grain growth were used iteratively to inform each subsequent stage of simulation. The model was then applied to predict the grain structure evolution during multiple-pass hot rolling of U-10Mo, and benchmarked against experimentally observed U-10Mo recrystallization behavior. The results showed that our model is able to capture the coupling between deformation and recrystallization, and quantitatively reproduce the observed U-10Mo recrystallization and grain growth kinetics with respect to time and temperature. A separate model of post-recrystallization U-10Mo grain growth is also discussed.

Research on Residual Stress Prediction and Regulation of 7050 Aluminum Alloy Thick Plate during Production Process: *Wang Junqiang*[1]; Yang Zhongyu[1]; Niu Guanmei[1]; Cao Hailong[1]; Liu Cheng[1]; [1]Chinalco Materials Application Research Institute Co., LTD

Large-scale structural parts are widely used in aircraft components. Residual stress of aluminum alloy thick plates is the cause of deformation. In this research, residual stress prediction and control technology of aluminum alloy thick plate was carried out by the prediction of quenching and pre-stretching process using finite element method (FEM) and the prediction of residual stress effect on machining deformation. The relationship between process parameters and residual stress, and the interaction between residual stress and processing deformation were obtained. Results showed that the heat exchange coefficient of surface in the range of 150~250°C had the closest influence on the residual stress during quenching process and the residual stress decreased with the increase in pre-stretching. According to the relationship between residual stress and machining deformation, a method of evaluating residual stress named “Cutting slit warping method” was developed, which was verified by 30~200mm plate.

Robust Integrated Design and Manufacturing Analysis of Composite Structures: Soban Babu Beemaraj[1]; Rizwan Pathan[1]; Yagnik Kalariya[1]; *Amit Salvi*[1]; [1]Tata Consultancy Services

Material selection for composite structures depends on many factors. Typical selection of such materials heavily depends on manufacturers' offerings and associated uncertainties. Mechanical properties of these materials are highly process dependent and uncertainties associated with these needs to be incorporated in the design process. The materials selected for the structure also needs to take into account the damage and repairs during its lifetime. This study details the inductive design exploration methodology in selection of robust materials by integrating design, manufacturing, and structural reliability. A 10 m long wind turbine blade(WTB) is designed under ICME paradigm. Robust material selection for the WTB is carried out by incorporating uncertainties in design. Selected material and design were analysed using Finite Element Analysis. IEC 61400 standard load cases were considered during the design. The designed WTB is subjected to manufacturing analysis as well as unexpected damage and corresponding repairs.

Role of Defects, Interfaces in FCC-BCC Massive Transformation in Iron Using Molecular Dynamics Simulation: *Pawan Tripathi*[1]; Somnath Bhowmick[1]; [1]IIT Kanpur

Austenite(FCC) to ferrite(BCC) transformation in iron is of great significance as it plays an important role in determining the microstructure and subsequently material properties. In the present work, the massive transformation from high temperature(FCC) phase to low temperature(BCC) phase is simulated using MD simulation. The simulations are performed by creating an FCC region, sandwiched between two BCC regions (interface formed according to Nishiyama-Wasserman orientation relationship, with (110) of BCC oriented parallel to (111) of FCC) in temperature range of 1000 to 1200 K. Orientation between the FCC and BCC phase was changed via tilting [111] direction of the FCC with respect to the [110] of the BCC region and is found to play a major role in transformation kinetics. We found that higher the misorientation, faster is the interface velocity (1.19 - 4.67 m/s) and mobility. Effect of point defects on massive transformation along with boundary defects was also analysed.

Self-consistent Model for Crack Propagation in Crystal Plasticity Using Concurrent Atomistic-CPFE Framework: *Subhendu Chakraborty*[1]; Somnath Ghosh[1]; [1]Johns Hopkins University, Baltimore

Atomistic-continuum concurrent multiscale models are widely used to assess the deformation mechanisms of materials. Very recently, a self-consistent concurrent atomistic-continuum model for finite temperature has been developed to study the elastic crack propagation in a Nickel single crystal [1]. In this present work, this model is extended to incorporate the plastic capability for both the domains. Once nucleated, dislocations propagate towards the interface. At the interface region dislocations are characterized and converted from their discrete representation to the density form. A 'generation-annihilation' mechanism is developed to make this incoming dislocation flux propagate in the continuum domain. The model is used to study and parametrize the evolution of plastic state variables during inhomogeneous deformation of a nickel single crystal owing to the presence of a crack inside the grain. This model is further used to construct the energy functional of phase-field model.[1] S. Ghosh and J. Zhang, IJF, 208:171-189 (2017).

Simulation and Characterization for Novel Metal Nanomaterials and Heterostructures: *Rongming Wang*[1]; [1]Beijing Advanced Innovation Center of Materials Genome Engineering, and Beijing Key Laboratory for Magneto-Photoelectrical Composite and Interface Science, School of Mathematics and Physics, University of Science and Technology Beijing

Simulation and characterization at nanoscale have enabled the discovery of many novel functional materials which started from understanding important relationships between material properties and structures. Here we demonstrate the research of structure stability of bimetallic nanocrystals and heterostructures at atomic scale. Pt-Au/C catalysts were synthesized with an ultrasound-assisted method. The extraordinary formic acid electrooxidation catalytic performance is attributed to the optimized synergistic effect of Pt and Au. The neighboring Au decreases the reaction energy barriers of the direct pathway on Pt. Au nanoparticles (NPs) with optimized size and distribution were deposited on few-layer MoS2 by e-beam evaporation firstly. A transition from Au nanoparticles to Au dendrites was observed when the as-prepared sample was irradiated by the high-energy electron beam in a transmission electron microscope. The atom-resolved morphology and structure evolution of Au NPs/MoS2 in this alignment process was investigated.

Simulation and Experiment Study on the Influence of Superimposed High-intensity Ultrasonic Vibration in Two Directions During ECAP: *Saeed Bagherzadeh*[1]; Qingyou Han[1]; Karen Abrinia[2]; [1]Purdue University; [2]University of Tehran

The application of high-intensity ultrasonic vibration in material forming especially in severe plastic deformation (SPD) methods has been grown as an emerging technique to improve SPD limitations. The ultrasonic vibration equal channel angular pressing (UV-ECAP) process was introduced to enhance mechanical properties and microstructure characterization of bulk materials as well as enhancing process parameters. In this research, a numerical-experimental study has been done to investigate the effect of applying vibration in two different directions as lateral or normal to the extrusion direction during the UV-ECAP process on aluminum grade 1050. A finite element model was developed with considering acoustic softening effect and the model is validated by UV-ECAP tests on the fabricated setup. Results showed that applying ultrasonic vibration in different amplitudes as normal vibration was more effective in comparison with the lateral vibration method on enhancing mechanical properties, grain refinement and improving process parameters in the UV-ECAP process.

Spectral Homogenization Approach for Precipitation-hardened Shape Memory Alloy Design: Aitor Cruzado[1]; *Jobin K. Joy*[1]; Alexandros Solomou[1]; Amine A. Benzerga[1]; Dimitris C. Lagoudas[1]; [1]Texas A&M University

Certain heat treatments of NiTi Shape Memory Alloys (SMAs) result in precipitation, which plays an important role in the effective shape memory response. Thus, a full-field based micromechanical model may be essential for predicting the effective nonlinear behavior. This implies microstructure-based computational homogenization of a 3D representative volume element (RVE), large enough to capture the effective behavior. A Fast Fourier Transform variational framework is developed which enables efficient solution to the non-linear system of governing equations. Comparisons with non-linear FEA methodologies are pursued. Determining the optimum RVE size, however, is a longstanding challenge. Here, we report on analyses of RVEs with varying number of particles and volume fraction. Focus is laid on defining a relation for RVE size in terms of the volume fraction of precipitates for a desired accuracy in the response. The computational efficiency derived from this FFT-homogenization approach is a step toward efficient high-throughput design of SMAs.

SPS of Al-CNTs-Nb Nano Composite for Power Transmission Conductor Core: *Chika Ujah*[1]; Patricia Popoola[1]; Olawale Popoola[1]; [1]Tshwane University of Technology

In powder metallurgy, conventional sintering always experiences grain growth and pore formations which result in the depreciation of both physical and chemical properties of the product. Spark Plasma Sintering (SPS) has the potentials of addressing these challenges. The bulk nature of Aluminium can be partially modified by the addition of a small amount of reinforcement to alter the matrix thus producing an advanced material with superior properties. Hence, this work involves SPS of Aluminium-Carbon nanotubes-Niobium nanocomposite and its characterisation for application in power transmission conductor core. Taguchi method was used to design the experiment. As-received nanopowders were mixed with tubular mixer and sintered with SPS machine. The thermal characterisation was conducted with Thermogravimetric Analyser; the Electrical conductivity was measured with a Four-Point Probe meter. Results were analysed with ANOVA and regression equations generated. Al-8CNTs-8Nb was thermally stable at 562°C; while the electrical conductivity increased from 0.224MS/m to 0.230MS/m.

Strengthening Effect due to Solid Solution and Short Range Ordering in High Entropy Alloys using Molecular Dynamics Simulations: *Shashank Mishra*[1]; Soumyadipta Maiti[1]; Beena Rai[1]; [1]Tata Consultancy Services Ltd.

High-entropy alloys (HEAs) have gained importance in recent times due to their exceptional structural and functional properties such as high temperature applications, wear resistant, corrosion resistant alloys, cryogenic, nuclear and biomedical applications etc. Experimental studies on body-centered cubic Hf-Nb-Ta-Zr HEA revealed formation of short-range ordering (SRO) in the system during annealing. In this work, the effect of these nano-scale SRO structures on the mechanical properties of the alloy has been studied using molecular dynamics. Critical resolved shear stress (CRSS) was estimated for pure elements, random solid solution and ordered solid solutions structures respectively by introducing an edge dislocation in these structures and compared with experiments. Simulations showed increased strengthening of the alloy due to presence of SRO in the structure (in <1 0 0> crystallographic directions) and the results were also semi-quantitatively validated against available experimental results, linking the mechanical properties of HEAs to their local structures.

Structural Evolution during Solidification Of Zr50Nb50 by Molecular Dynamics Simulation: *Asefa Frew*[1]; [1]Jimma University

The local atomic structure evolution of Zr50 Nb50 melt was studied at different temperatures by employing classical molecular dynamics simulations. In order to get clear insight into the structural evolution during quenching, we used various structural analysis methods such as the radial distribution function g(r), coordination number, HA indices,and Voronoi tessellation analysis. We found that the icosahedral motifs (which is the sig-nature of short-range ordering) dominate in the liquid and super-cooled region before the system undergoes a first-order transformation at about 1000K. Upon further decreasing the temperature, all the structural analysis show that the system solidifies with majority of body centered cubic-like clusters in the case our specific cooling rate 1011 K/S .

Study of Brittle Film Induced Cracking of Ductile Substrate Based on High Throughput Technique: *Xiaolu Pang*[1]; [1]University of Science and Technology Beijing

By depositing TiN flm on the lateral surface of the stainless substrate and loaded in three-point bending to the maximum normal strain of 6%, different stress state was obtained according to the distance to the neutral axis. We used high throughput XRD technique to characterize the stress evolution along the film growth direction under different tensile stress state. In addition, the cracking behaviors and their effect on the underlying substrate were also studied during high throughput experiments. It shown that the tensile stress was the maximum at the middle of the film depth, where the cracks initiated. The cracking of TiN film caused the fracture of stainless substrate, which decreased the ductility and fatigue life of the substrates. This high throughput technique provides a new method for us to study the failure of film-substrate system efficiently.

The Application of Deep Learning in Statistical Dendritic Spacing: *Weihao Wan*[1]; DongLing Li[1]; HaiZhou Wang[1]; Lei Zhao[1]; XueJing Shen[1]; Qian Wu[2]; [1]China Iron and Steel Research Institute; [2]Other

Dendritic structure is a characteristic structure produced during the directional solidification of metal materials. Primary dendrite arm spacing is an important characteristic parameter of dendritic structure. This paper combines image processing and deep learning to accurately locate the center position of the dendrites, and mathematically calculates the distance between each dendrite and the nearest dendrites in all directions. First, the images are pre-processed by image processing, the positions of the dendrites are pre-judged and the pre-judgment results are marked. Then, the pre-judgment results are judged manually as the final labels, which are divided into a training set and a test set. The training set is trained by deep learning, and the training result will be verified by test data. Experiments show that the accuracy of the method in determining the position of the dendrites can reach 94%.There will be no manual intervention in the testing process.

The Development of the SIP-MI System for Structural Materials: *Satoshi Minamoto*[1]; Takuya Kadohira[1]; Kaita Ito[1]; Makoto Watanabe[1]; Masahiko Demura[1]; [1]National Institute for Materials Science

Materials Integration (MI) System, a web-based tool to analyze material performance such as fatigue life limit or creep damage, was developed in Japanese Cross-ministerial Strategic Innovation Promotion Program (SIP). In this system, it is intended to solve the problems of structural materials composed by various inputs and outputs by combing the four sciences of theory, experiment, calculation, and data science. Practically, by combining different kinds of computer programs (numerical calculation, database, machine learning, etc.), it aims to understand the performance on structural materials. As merits of constructing coupled models (workflow), there are objectification of problems and calculation being automated. By performing many evaluations of workflows, huge amount of data is generated, and it is possible to construct reusable machine learning models. Then user can calculate in multi-scale while concentrating on the calculations of interest for important problems concerning the performance of structural materials.

Three-dimensional Imaging of Hydrogen Distribution in Titanium Alloys by Neutron Tomography: *Lixia Yang*[1]; Danqi Huang[2]; Lei Zhao[1]; Xuejing Shen[1]; Haizhou Wang[1]; [1]China Iron and Steel Research Institute; [2]University of Science and Technology Beijing

Titanium alloys play significant roles in aerospace, biomedical and chemical industries. Thermohydrogen processing (THP) offers an effective method for improving the workability and deformability of titanium alloys via high temperature hydrogenation treatment. Further optimization of THP process requires an comprehensive understanding of relationship of microstructure, properties and hydrogen distribution of titanium alloys. In this work, the hydrogen distributions were observed by neutron tomography. Cold neutrons were provides by the research BER II to picture the samples with a spatial resolution in the reconstructed three-dimensional model of ~57 µm. We made the unique observation that hydrogen content decreased from the edge to the center of samples. The content of ß phase rised with the increase of hydrogen content according to the full field machine learning and statistical analysis. Some acicular structure appeared and hydrides were formed at high hydrogen content zone. The mechanical properties also changed with different hydrogen content.

Towards Building Machine Learning Tools for High Strain Rate, High Temperature Deformation of Carbon Steels: *Shengyen Li*[1]; Steven Mates[2]; Mark Stoudt[2]; Carelyn Campbell[2]; [1]Southwest Research Institute; [2]National Institute of Standards and Technology

A Python-based machine-learning (ML) workflow is developed to understand the non-equilibrium behavior of carbon steels during a Kolsky Bar experiment, where rapid heating followed by deformation then rapid cooling produce unexpected microstructures and material behavior. For this application, it is important to predict the volume fraction and the stability of the austenite phase as function of the thermal and deformation processes. This work combines scanning electron microscopy, high rate deformation data, and the reference data with a ML model to assess the austenite stability. This ML model incorporates the physics from Ghosh-Olson model and the mathematical formulas are selected by data and cross-validation process. A power law function uses the microstructure and testing conditions to calculate the stress-strain curves. The parameterization of this power-law model is determined by another set of ML models. A comparison of the predicted phase transformations and stress-strain curves to the experimental observations will be presented.

Understanding the Core-shell Coupling Effect in an Oxygen Evolution Reaction Catalyst: *Yingying Xu*[1]; Rongming Wang[1]; [1]Beijing Advanced Innovation Center of Materials Genome Engineering, and Beijing Key Laboratory for Magneto-Photoelectrical Composite and Interface Science, School of Mathematics and Physics, University of Science and Technology Beijing

The development of oxygen evolution reaction (OER) catalysts with high catalytic performance based on inexpensive materials has become a key part of hydrogen energy applications. With the fine control of the structure and morphology, we successfully prepared Au-Ni12P5 core-shell nanostructure with good OER catalytic performance. Weak electrostatic potential distribution and the covalent bonding nature of Ni-P were revealed, which might explain the relatively weak adsorption sites at the Ni12P5 surface which favor good OER activity. Compared with pure Ni12P5 nanoparticles (NPs) and Au-Ni12P5 oligomer-like NPs, the core/shell crystalline structure with Au shows improved OER activity. This enhanced OER activity may be related to the effective structural and electric coupling between the single-crystal Au core and overlaid semiconductor shell.

Variant Selection of Intragranular Ni2(Mo,Cr) Precipitates in the Ni-Mo-Cr-W Alloy: *Yao Fu*[1]; [1]University of Cincinnati

Variant selection of Ni2(Mo,Cr) precipitates in a Ni-Mo-Cr-W alloy has been investigated as a function of precipitate size and applied stress. The lenticular-shaped, coherent precipitates form with a {110}M/(010)p habit plane. During conventional aging, all 6 variants of the Ni2(Mo,Cr) precipitates form and coarsen with aging time. With the application of external loading below the yield stress during aging, variants with {110}M habit planes that experience the largest dilations resulting from the externally applied stress are favored. Phase field modeling has been employed to simulate the development of variant selection of gamma prime precipitates with and without applied external loading. Similar to the experimental results, the gamma prime precipitates tend to form parallel to each other during coarsening and display variant selection when external stress is applied during aging. The mechanism is believed to be the reduction of elastic strain energy caused by the precipitate/matrix lattice mismatch.

A Digital Representation of a Microstructure and Determining Its Mechanical Behavior: *Burak Bal*[1]; [1]Abdullah Gül University

Mechanical characterization tests might come with a remarkable cost of time and money for both companies and academics. The inquiry to transform laboratory experiments to the computational media is getting a trend; accordingly, the literature supplies many analytical ways to explain the mechanics of deformation. In our work, we focused on the crystal plasticity finite element modeling (CPFEM) analysis on various materials in various crystal structures to predict the stress-strain curve without tensile tests. For FEM analysis, which we used in this study was ABAQUS, a standard user defined material subroutine (UMAT) was prepared. The geometry of a specimen was created via DREAM 3D software with the inputs of Euler angles taken by Electron Back-Scattered Diffraction (EBSD) technique as orientation, or misorientation angles. The synthetic crystal created with DREAM 3D is also meshed in a way the grains inside the crystal meshed separately, and the computer can realize interaction of inter, and intra grain structures. The mechanical deformation parameters obtained from the literature put into the Fortran based UMAT code to describe how material will response to the load applied from specific direction. The mechanical response of a synthetic crystal created with DREAM 3D agrees well with the material response in the literature.

Simulation of Two-dimensional Diffusion and Kirkendall Shift in Single-phase Diffusion Triples: Cheng-Hui Xia[1]; *Shi-Lin Xia*[1]; Xiao-Gang Lu[1]; Ying Li[1]; [1]Shanghai University

Diffusion simulation is a key link in ICME for engineering materials.Two-dimensional (2D) diffusion process controlled by Fick's laws has been successfully simulated by a fully discrete local discontinuous Galerkin (LDG) method, which has advantages in dealing with strong discontinuity problems. Reliability of simulation results was proved by using ternary Co-Fe-Ni diffusion triple experiments. The traditional simulation software based on thermodynamic and diffusion kinetic databases can only tackle one-dimensional (1D) diffusion problems. It cannot handle composition gradients in two independent directions. However, our simulation code using LDG method combining with thermodynamic and diffusion kinetic databases can deal with this problem easily. In addition, this code can effectively track the movement of Kirkendall plane in 2D single-phase diffusion zone, while the traditional graphic method fails.

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