TMS The Mineral, Metals & Materials Society Presents:

The 3rd International Congress on 3DMS

3D Materials Science 2016

July 10–13, 2016 • Pheasant Run Resort • St. Charles, Illinois, USA

FINAL PROGRAM

Sponsored by:

TMS The Minerals, Metals & Materials Society and the TMS Advanced Characterization, Testing & Simulation Committee

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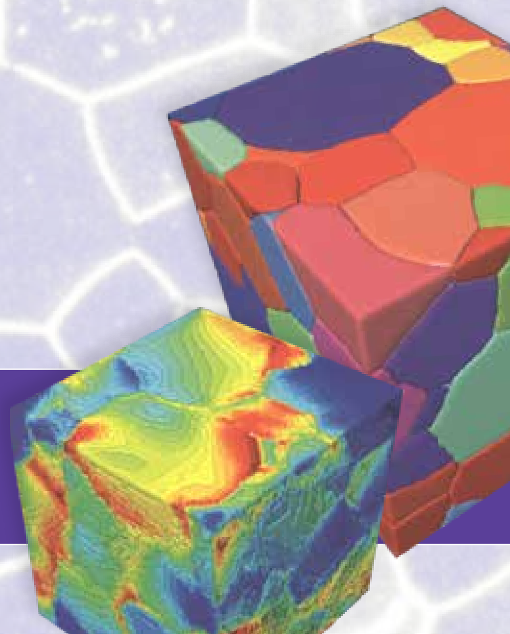

WELCOME TO

The 3rd International Congress on

3DMS

3D Materials Science 2016

On behalf of The Minerals, Metals & Materials Society (TMS) and the congress organizers, I am pleased to welcome you to the third iteration of the International Congress on 3D Materials Science (3DMS 2016). This multi-disciplinary meeting distills the most current knowledge regarding 3D materials science into one conference, enabling you to fast forward your materials research impact. I hope you will take every opportunity during this week to immerse yourself in this unique, highly focused technical meeting where you have the chance to learn from and network with other 3D materials science experts. The 3DMS 2016 technical program will include plenary and invited lectures as well as oral and poster presentations including a wide range of topics areas, covering the most critical and rapidly growing areas of 3D materials science.

I look forward to an exciting congress and thank you for your participation in 3DMS 2016!

Warmest regards on behalf of the Organizing Committee.

ORGANIZING COMMITTEE

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SCHEDULE OF EVENTS & TABLE OF CONTENTS

Date	Function	Time	Location
Sunday, July 10	Registration	5:00 p.m. to 7:30 p.m.	St. Charles Ballroom Lobby
	Welcome Reception	6:30 p.m. to 7:30 p.m.	New Orleans Ballroom
Monday, July 11	Registration	7:00 a.m. to 6:00 p.m.	St. Charles Ballroom Lobby
	Session: Plenary	8:00 a.m. to 9:00 a.m.	St. Charles Ballroom Salons III & IV
	Break	9:00 a.m. to 9:10 a.m.	St. Charles Ballroom Lobby
	Technical Sessions	9:10 a.m. to 12:00 p.m.	see pages 8-10 for locations
	Exhibition Set-Up	10:00 a.m. to 2:00 p.m.	St. Charles Ballroom Salon II
	Break	10:20 a.m. to 10:40 a.m.	St. Charles Ballroom Lobby
	Lunch	12:00 p.m. to 2:00 p.m.	On Your Own
	Technical Sessions	2:00 p.m. to 3:00 p.m.	see pages 10-11 for locations
	Exhibition	3:00 p.m. to 5:00 p.m.	St. Charles Ballroom Salon V & VI
	Poster Viewing/ Networking Reception	3:10 p.m. to 4:40 p.m.	St. Charles Ballroom Salon V & VI
	Technical Sessions	4:40 p.m. to 6:10 p.m.	see pages 11-24 for locations
Tuesday, July 12	Registration	7:30 a.m. to 6:30 p.m.	St. Charles Ballroom Lobby
	Session: Plenary	8:00 a.m. to 9:00 a.m.	St. Charles Ballroom Salons III & IV
	Exhibition	8:00 a.m. to 5:00 p.m.	St. Charles Ballroom Salon V & VI
	Break	9:00 a.m. to 9:10 a.m.	St. Charles Ballroom Salon V & VI
	Technical Sessions	9:10 a.m. to 12:20 p.m.	see pages 24-26 for locations
	Break	10:20 a.m. to 10:40 a.m.	St. Charles Ballroom Salon V & VI
	Lunch	12:20 p.m. to 2:00 p.m.	On Your Own
	Technical Sessions	2:00 p.m. to 3:50 p.m.	see pages 26-28 for locations
	Break and Vendor Showcase	3:50 p.m. to 4:50 p.m.	St. Charles Ballroom Salon III
	Technical Sessions	4:50 p.m. to 6:10 p.m.	see pages 28-30 for locations
	Congress Dinner	6:30 p.m. to 8:30 p.m.	Pool Deck (Weather Permitting)
Wednesday, July 13	Registration	7:30 a.m. to 4:30 p.m.	St. Charles Ballroom Lobby
	Exhibition	8:00 a.m. to 3:30 p.m.	St. Charles Ballroom Salon V & VI
	Technical Sessions	8:00 a.m. to 12:00 p.m.	see pages 30-32 for locations
	Break	9:30 a.m. to 10:00 a.m.	St. Charles Ballroom Salon V & VI
	Lunch	12:00 p.m. to 2:00 p.m.	On Your Own
	Technical Sessions	2:00 p.m. to 3:10 p.m.	see pages 32-33 for locations
	Break	3:10 p.m. to 3:30 p.m.	St. Charles Ballroom Salon V & VI
	Exhibition Dismantle	After 3:30 p.m.	St. Charles Ballroom Salon II
	Panel Discussion	3:30 p.m. to 5:00 p.m.	St. Charles Ballroom Salons III & IV

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REGISTRATION

Your registration badge ensures admission to each of these events:

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

Registration Hours

The registration desk will be located in the St. Charles Ballroom Lobby.

Sunday	5:00 p.m. to 7:30 p.m.
Monday	7:00 a.m. to 6:00 p.m.
Tuesday	7:30 a.m. to 6:30 p.m.
Wednesday	7:30 a.m. to 4:30 p.m.

Internet Access

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

Technical Sessions

All oral presentations will be held in the St. Charles Ballroom Salon III and IV of the Pheasant Run Resort. All poster presentations will be held in St. Charles Ballroom Salon V and VI. See the Technical Program section on pages 7-33 for room locations.

Exhibition Hours

The exhibition will be located in St. Charles Ballroom Salon V and VI.

Monday	3:00 p.m. to 5:00 p.m.
Tuesday	8:00 a.m. to 5:00 p.m.
Wednesday	8:00 a.m. to 3:30 p.m.

ABOUT THE CONGRESS

NETWORKING & SOCIAL EVENTS

Welcome Reception

The Welcome Reception will be held on Sunday, July 10 from 6:30 p.m. to 7:30 p.m. in the New Orleans Ballroom.

Poster Viewing/Networking Reception

A Networking Reception is planned for Monday, July 11 from 3:10 p.m. to 4:40 p.m. in St. Charles Ballroom Salon V & VI. Don't miss this great networking opportunity!

Congress Dinner

The dinner will be held on Tuesday, July 12 from 6:30 p.m. to 8:30 p.m. on the pool deck. Weather permitting, of course.

PLENARY SPEAKERS

Jonathan Almer
Argonne National Laboratory, USA

Paul Dawson
Cornell University, USA

ABOUT THE VENUE

Pheasant Run Resort
Conveniently located in peaceful St. Charles, about one hour outside of downtown Chicago, the 250-acre country property is one of the largest entertainment, conference center, and family vacation resorts in the Midwest. The Pheasant Run Resort is practically a city itself, with everything you need including a theater, live comedy, diverse dining options, 18 holes of golf, tennis, and swimming. For more information, visit www.pheasantrun.com.

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

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SILVER SPONSOR

FEI
FEI will present Avizo - an advanced 3D visualization and analysis software solution widely employed in Material Sciences. Avizo is the ideal tool for characterizing materials' structures, properties and performance, in a wide range of applications (porous media, metals and alloys, fibrous materials, composites …). From state of the art visualization and measurement to advanced image processing, quantification, analysis and reporting, Avizo provides a comprehensive, multimodality digital lab for advanced 2D and 3D materials characterization.

BRONZE SPONSOR

UES
Robo-Met.3D: 3D Material Characterization, a UES Product
Robo-Met.3D is an automated serial sectioning system generating 2D microstructural data for 3D characterization. High resolution three dimensional investigation of: grain size, grain shape, porosity, pore interconnectivity, cracks and failure points. Robo-Met.3D applications include; Petrology porosity analysis, Aerospace materials characterization, Automotive cast components and Coatings Analysis. As demonstrated in the image, relying upon 2D image analysis would have resulted in miscalculating porosity by more than 50%. Contact tkielbaso@ues.com / 937-426-6900 for more information.

EXHIBITORS

Micro Photonics Inc.
Micro Photonics Inc., and partner Bruker MicroCT, are leading the advancement in high resolution nano- & micro-CT solutions for materials science research. Bruker's SkyScan Micro-CTs meet the 3D high-resolution and versatility required for any demanding research laboratory. Micro Photonics offers contract testing services and system sales for Bruker Micro-CTs.

Simpleware
Simpleware provides software and services for converting 3D image data (MRI, CT, micro-CT…) into high-quality models for CAD, CAE and 3D Printing. Simpleware software enables comprehensive image visualisation, analysis and model generation from scan data, ensuring accurate reconstruction of complex natural and man-made structures. The software is used for applications in the Life Sciences, Materials Science, Industrial Non-Destructive Evaluation and Reverse Engineering, 3D Printing, Oil and Gas, and any field involving 3D image data.

VENDOR SHOWCASE

Tuesday, July 12 • St. Charles Ballroom Salon III

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

3:50 p.m.: Simpleware
4:00 p.m.: Carl Zeiss Microscopy, LLC
4:10 p.m.: UES
4:20 p.m.: Micro Photonics Inc.
4:30 p.m.: FEI

CONGRESS POLICIES & INFORMATION

MEETING POLICIES

Badges

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

Refunds

The deadline for all refunds was June 10, 2016. No refunds will be issued at the congress. Fees and tickets are nonrefundable.

Americans with Disabilities Act

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

Cell Phone Use

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

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

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

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Antitrust Compliance

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

STAY FOR THE WORKSHOP!

Methods and Software Tools for 3D Microstructural Science

Thursday, July 14–Friday, July 15
Pheasant Run Resort • St. Charles, Illinois, USA

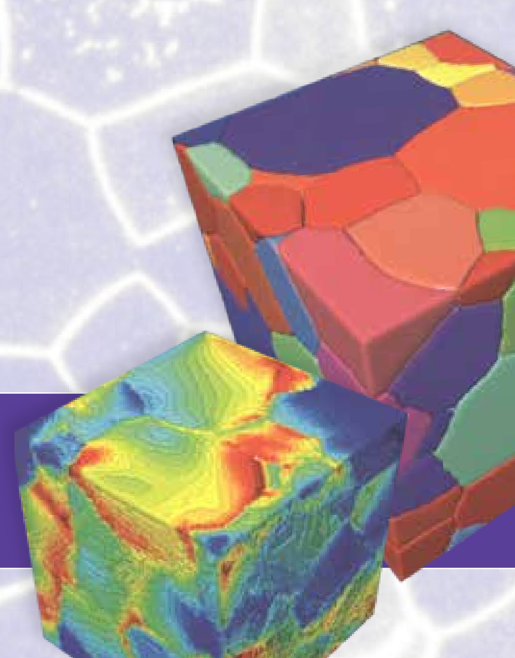
Stop by the registration desk (located in the St. Charles Ballroom Lobby) to register for the workshop and enhance your congress experience.

The 3rd International Congress on

3DMS

3D Materials Science 2016

TECHNICAL PROGRAM



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Plenary 1

Monday AM Room: Salons III&IV
July 11, 2016 Location: Pheasant Run Resort

8:00 AM Plenary
Developing Principle-Based Approaches to Quantify Mechanical Property Distributions of Titanium Alloys: *Paul Dawson*[1]; [1]Cornell University

A long-standing goal of the materials science and mechanics communities is develop a principle-base approach to estimate an alloy's aggregate properties from knowledge of its mi-crostructural state, the local properties of its constituent phases, and the type of loading being applied. A combination of experimental and modeling capabilities have emerged over the past decade that provide practical tools to reach this goal. From the experimental side, these include electron and x-ray diffraction methods for quantifying microstructures of polyphase, polycrys-talline alloys and for measuring mechanical behaviors at the scale of individual grains. From the simulation side, these include tools to instantiate virtual samples that adequately replicate mea- sured microstructures and parallel finite element formulations capable of dealing with complex behaviors. In this presentation, I discuss a multi-investigator project with the goal of coordinating these capabilities to estimate distributions of strength and ductility in a two-phase titanium alloy (Ti-6Al-4V) that has been processed to achieve distinctly different microstructures. Em- phasis is placed on new analytical tools that have been developed to more effectively integrate together the data from the different sources and to reduce uncertainties in critical input param- eters used in simulating the mechanical behavior. In closing, I'll discuss a few challenges that persist and offer interesting opportunities for continued research.

9:00 AM Break

Advances in 3D Materials Modeling: Deformation Modeling of Metallic Alloys

Monday AM Room: Salon III
July 11, 2016 Location: Pheasant Run Resort

Session Chairs: Armand Beaudoin, University of Illinois at Urbana-Champaign; Paul Dawson, Cornell University

9:10 AM Invited
Crack Deviation in an Aluminum Alloy for Structural Aerospace Application: *Armand Beaudoin*[1]; Kamalika Chatterjee[1]; Robert Dodds[1]; Peter Kenesei[2]; Jun-Sang Park[2]; Sarvjit Shastri[2]; [1]University of Illinois at Urbana-Champaign; [2]Argonne National Laboratory

Complex structural aerospace components are high-speed machined out of (thick) hard aluminum alloy plate. Demand for increased performance and reduced weight leads to complex loading scenarios and consequent development of localized stress states that drive microstructure-related mechanisms of failure. High-energy x-ray diffraction (HEXD) and modeling are combined to provide insight into crack deviation in AA 7050 hard alloy plate. A far-field diffraction geometry utilizing a high resolution monochromator and line focus beam is applied to evaluate lattice strain at the subgrain scale in a notched sample geometry. Distinct lattice orientations exhibiting large differences in strain -- observed through HEXD -- are then used to initialize a model of a crack in a pancake-grain microstructure. The model is built upon the code Warp3d. The simulation reveals driving forces for crack deviation that are in line with experimental observations.

9:40 AM
Image-Based Finite Element Analysis of Ductile Fracture via Hydrogen Pore Mechanism in an Aluminum Alloy: *Akihide Hosokawa*[1]; Hiroyuki Toda[2]; Rafael Batres[3]; Osamu Kuwazuru[4]; Masakazu Kobayashi[5]; Han Li[2]; Hidetaka Yakita[2]; [1]National Institute of Advanced Science and Technology; [2]Kyushu University; [3]Tecnológico de Monterrey; [4]The University of Fukui; [5]Toyohashi University of Technology

Finite element analyses based on 3D images of the microstructure in an aluminum alloy observed by X-ray microtomography (so called image-based finite element analysis = IB-FEA) were performed to assess the influences of microstructures on ductile fracture behavior. The exact microstructural features of the aluminum alloy (i.e. hydrogen pores and particles) were perfectly reproduced in the FE models. The microstructural parameters (e.g. diameter, sphericity, volume of pores/particles) were quantified through a handmade software. IB-FEA provided indirect measure of ductility (or risk of ductile fracture), extracting the damage-/fracture-related values (e.g. maximum principal stress, stress triaxiality and equivalent plastic strain) through J_2 plasticity simulations. This made it possible to discuss the microstructure-ductility relationship. Data mining was performed to filter out the microstructural parameters that do not contribute to ductility. An attempt to optimize microstructure using a surrogate model will be demonstrated in the presentation.

10:00 AM
Direct Numerical Simulation (DNS) of Failure Mechanisms in Brittle Polycrystalline Structures: *Bo Li*[1]; Jiang Hao[1]; [1]Case Western Reserve University

We propose an image based computational tool for the direct numerical simulation (DNS) of polycrystalline structures using the Finite Element method. The DNS model is initialized using the probability distribution functions (PDF) of grain sizes, orientations and misorientation from 3D microstructural characterization. Grain boundaries are explicitly modeled by elements with non-zero misorientation angles. In addition, the EigenErosion algorithm is employed to predict the fracture propagation in polycrystalline structures. In this method, an equivalent energy release rate is defined at the elements to evaluate the local failure state by comparing to the critical energy release rate, which varies at the grain boundaries and the interior of grains. As a consequence, the DNS model is capable of predicting the dynamic strength of brittle materials dominated by a combination and competition of intergranular and transgranular fracture patterns. The model is validated against Split Hopkinson Pressure Bar experiments on the compressive strength of SiC.

10:20 AM Break

10:40 AM
3D Characterization of Inhomogeneous Deformation in Grain Microstructure of Aluminum Alloy: *Masakazu Kobayashi*[1]; Aya Kouno[1]; Tomohiko Matsuyama[1]; Hiroyuki Toda[2]; Hiromi Miura[1]; Osamu Kuwazuru[3]; [1]Toyohashi University of Technology; [2]Kyushu University; [3]Fukui University

Inhomogeneous deformation of grain microstructure is one of important issue, because the inhomogeneity concerns the origins of yielding, fracture and recrystallization. In this study, 3D plastic strains during tensile deformation and grains shapes have been investigated by using synchrotron X-ray microtomography. Further, image-based grain microstructure models for crystal-plasticity finite element analysis have been developed to understand effects of neighbor crystallographic orientation and grain shapes on inhomogeneous deformation.

11:00 AM
Non-destructive 3D Microstructure Measurement and Mechanical Deformation Modeling of Additively Manufactured Materials: *Tugce Ozturk*[1]; Ross Cunningham[1]; David Menasche[1]; Robert Suter[1]; Anthony Rollett[1]; [1]Carnegie Mellon University

Additive manufacturing is increasingly being implemented to structural components, yet the microstructural evolution and resulting mechanical properties are still work in progress. The purpose of this study is to combine the 3D experimental and computational methods for the evaluation of structure-property relationship of these materials. In order to measure the process dependent grain structure characteristics non-destructively, high-energy X-ray diffraction microscopy is performed on AM parts. Measured microstructures are used to validate the synthetic microstructure reconstruction, and these structures are used in the computational calculations via the Fast Fourier Transform (FFT) based full field technique in the elastic, viscoplastic and elasto-viscoplastic deformation regimes, to meticulously study the effect of microstructural features such as the prior-beta grain size, primary-alpha colony size, the size and shape of the primary-alpha grains and the volume fractions on the mechanical properties. The results help to link the processing parameters of AM and resulting multi-scale mechanical properties.

11:20 AM
Image-Based Finite Element Analysis for Fatigue of Cast Aluminum Alloy: *Osamu Kuwazuru*[1]; Masaki Teranishi[1]; Keigo Matsumura[1]; Shota Gennai[1]; Masakazu Kobayashi[2]; Hiroyuki Toda[3]; [1]University of Fukui; [2]Toyohashi University of Technology; [3]Kyushu University

The mechanism of fatigue crack initiation in cast aluminum alloys was addressed through the image-based micromechanical simulations. The low-cycle fatigue tests and the in situ CT observations were carried out in the synchrotron radiation facility SPring-8. From the chronological observation, the crack initiation site was identified, and a small size image around the initiation site was cut out from the initial CT image. The shape of inclusions such as silicon and intermetallic compound were extracted as a surface geometry data, and the finite elements were generated based on the geometry. The cyclic uniaxial loading was applied on the boundary of the finite element model. The material property of aluminum, silicon and intermetallic compounds were identified by the nanoindentation tests. From the simulation results, we found that the cyclic loading induced a gradual increase in the stress of silicon particles by the variation in the plastic strain in aluminum matrix.

11:40 AM
Examining Interactions between Microscale Deformation and 3D Microstructure in an \945-Titanium Alloy: *Zhe Chen*[1]; Samantha Daly[1]; [1]University of Michigan

Characterization of the three-dimensional microstructure is critical for understanding the mechanisms of heterogeneous deformation in materials. In the current study, multi-scale deformation behavior of \945-titanium alloys was investigated by an experimental approach combining several characterization techniques. The full-field deformation at the microstructural length scale was continuously tracked during *in-situ* mechanical testing by scanning electron microscopy. High resolution, distortion-corrected digital image correlation was performed to enable identification of individual slip traces over large areas covering hundreds of grains, which allowed for the extraction of statistical significant information through data mining. The three-dimensional microstructure was reconstructed by electron-backscattered diffraction (EBSD) and post-deformation serial sectioning. The effect of three-dimensional microstructural neighborhoods, such as grain dimensions and neighbor misorientation, on strain localization and the activity of different deformation systems was investigated through statistical learning approaches.

12:00 PM
Modeling, Analysis and Ultrafast Imaging of Lattice Dynamics in Core-Shell Bimetallic Nanocrystals: *Kiran Sasikumar*[1]; Mathew Cherukara[1]; Ross Harder[1]; Jesse Clark[2]; Nicola Ferrier[1]; Thomas Peterka[1]; Subramanian Sankaranarayanan[1]; [1]Argonne National Laboratory; [2]SLAC National Accelerator Laboratory

Investigation of the temporal behavior of externally stimulated materials, under ultrafast laser excitation, can lead to crucial insights for energy research. Recently, experimental techniques have evolved to conduct time-dependent lattice dynamics measurements in nanomaterials. Coherent Diffraction Imaging (CDI), in conjunction with optical pump-probe experiments via femtosecond x-ray lasers, has been used to directly image the evolution of coherent acoustic phonons within nanocrystals. In particular, experiments on bimetal (Au/Al) core-shell nanocrystals have revealed inhomogeneous effects in the lattice breathing upon laser heating. Conventional theoretical models fail to explain the physics of the phenomena in such non-equilibrium environments, particularly in core-shell structures where interfacial effects can play an important role in phonon scattering. Here, we discuss how multi-million atom molecular dynamics simulations are used to obtain x-ray diffraction patterns that are directly compared with CDI images to reveal the role of the interface in the lattice breathing of core-shell nanocrystals.

12:20 PM Lunch

Experimental Techniques for 3D Data Acquisition: Investigating Materials at the Nano and Dislocation Scale

Monday AM — Room: Salon IV
July 11, 2016 — Location: Pheasant Run Resort

Session Chairs: Satoshi Hata, Kyushu University; Henry Proudhon, MINES ParisTech

9:10 AM Invited
Advances in Experimental Techniques for 3D Dislocation Image Acquisition Using Electron Microscopy: *Satoshi Hata*[1]; [1]Kyushu University

After the first report on 3D dislocation imaging using electron tomography by Barnard et al. in 2006, several research groups have developed their own experimental techniques for 3D dislocation image acquisition. Although dislocations in a crystal can now be visualized in a 3D volume from a few images and an appropriate reconstruction algorithm, there would still be the effectiveness of conventional tilt-series acquisition for 3D dislocation imaging due to some practical aspects. Here, the author reports recent advances in his experimental techniques for 3D dislocation image acquisition using electron microscopy. The main topics are as follows: (i) new functions and applications of high-angle triple-axis specimen holders [Ultramicrosc. 111, 1168 (2011)] which are capable of precise diffraction alignments; (ii) experimental techniques for tilt-series acquisition for ferrous samples prepared by conventional electropolishing [ISIJ International 55, 623 (2015)]; (iii) 3D imaging of dislocations using a SEM-FIB slice-and-view technique [Scripta Mater. 101, 801 (2015)].

9:40 AM
Mapping of Embedded Dislocations in Diamond with Sub 200 nm Resolution: *Anders Jakobsen*[1]; Hugh Simons[1]; Sonja Ahl[1]; Carsten Detlefs[2]; Jürgen Härtwig[2]; Henning Poulsen[1]; [1]DTU Physics; [2]ESRF

We present the case of using dark field x-ray microscopy to map dislocations in 3D. With an angular resolution of ~5 µrad and a spatial resolution currently below 200 nm, the microscope can zoom in on an ensemble of embedded dislocations and provide 3D maps with a time resolution of order minutes. Furthermore, components of the strain field around the dislocations can be mapped, thereby revealing Burgers vectors. Effects of dynamical scattering are overcome by full field imaging and novel contrast methods. First results relate to a 17 keV study at the European Synchrotron Radiation Facility of dislocations within a 400 µm thick diamond sample. Potential applications are outlined.

10:00 AM
Dislocations Patterns in Plasticity: Formalism, Computational Algorithms and Connection with 3D X-Ray Microscopy: *Anter El-Azab*[1]; Shengxu Xia[1]; Bennett Larson[2]; [1]Purdue University; [2]ORNL

We present a continuum dislocation dynamics model for mesoscale plasticity that predicts the formation of dislocation cell structure under monotonic loading of copper, in conjunction with the famous similitude law for the dependence of cell size on stress, and the dislocation vein structure under cyclic loading. This model features dislocation transport equations coupled with crystal mechanics, plus a closure problem consisting of finding the spatial and temporal correlations of the dislocation system. Our approach has been used to obtain a full solution of the deformation problem, which includes the dislocation pattern, deformation pattern and distorted shape, internal elastic fields, and stress-strain response. The results reveal the critical role of cross slip in cell structure formation under monotonic loading, and the relative suppression of this role when cyclic loading is applied. We give a short review of the model along with a comparison of results with 3D X-ray microscopy data.

10:20 AM Break

10:40 AM
Mapping Nano-Scale Strain and Orientation in Multiferroic Materials with Dark-Field X-Ray Microscopy: *Hugh Simons*[1]; Sonja Ahl[1]; Anders Jakobsen[1]; John Daniels[2]; Dragan Damjanovic[3]; Carsten Detlefs[4]; Henning Poulsen[1]; [1]DTU; [2]University of New South Wales; [3]Swiss Federal Institute of Technology in Lausanne-EPFL; [4]The European Synchrotron - ESRF

Domain walls in multiferroic materials are subject to localised strain that can give rise to nano-scale conductivity, photoelectric effects and flexoelectricity. These effects are key to emerging devices such as memristors, high-density digital memory and self-writing electrical circuits. Yet, the subtlety of the strain fields and their sensitivity to external boundary effects makes the coupling between strain and domain topology difficult to measure. Here we use dark-field x-ray microscopy to non-destructively map strain and orientation around individual, embedded domain walls with spatial and orientation resolution of the order of 100 nm and 5 µrad, respectively. The technique presents a new way to directly observe the effects of domain walls on the local crystal structure without the spurious boundary effects that occur in thin samples and at surfaces. The resulting 3D orientation and strain maps can then be used to validate theoretical models of the material structure and functionality.

11:00 AM
Early Stage of Plastic Deformation in Metals Studied by In Situ X-Ray Synchrotron Topotomography and Crystal Plasticity FEM Simulations: *Nicolas Gueninchault*[1]; Henry Proudhon[1]; Wolfgang Ludwig[2]; Samuel Forest[1]; [1]Mines Paristech; [2]ESRF

In situ X-ray synchrotron topotomography on a 3-grains cluster within the bulk has been performed for the first time. Thanks to the specifically designed NANOX device, the very first plastic events in the individual grains have been captured. Single or multiple slip bands formation is observed depending on the grain orientation and load level. The 3D microstructure (grain shape and orientation) of the entire sample was characterized by diffraction contrast tomography. This reconstruction was used to generate a realistic mesh of the specimen and to perform crystal plasticity finite element simulations within the finite strain framework. Simulation results of the mechanical grain behaviour are directly ccompared to our experimental observations (rocking curves, grain rotation, plastic strain localization).

11:20 AM
Understanding Microplasticity Processes Related to Fatigue Damage using High Energy X-Rays and a Crystal-Based Modeling Formulation: *Mark Obstalecki*[1]; Robert Carson[1]; Paul Dawson[1]; Matthew Miller[1]; [1]Cornell University

Microcrack nucleation within ductile polycrystals during low cycle fatigue conditions is studied using high energy x-ray diffraction. Using synchrotron radiation, the rotating crystal method is employed to identify regions of heterogeneous cyclic slip within a polycrystalline aggregate. We hypothesize that during cyclic loading, the plastic strain is eventually localized into regions within individual grains. This localized cyclic deformation may lead to the formation of microcracks. Experimentally we determine each grain's center of mass position, orientation, average lattice strain, and lattice heterogeneity. Since the experimental technique does not provide us with information about spatial distributions within grains, we have created a combined experiment/ simulation methodology for tracking heterogeneous cyclic plasticity within grains. Details of the subgrain response such as the stress distribution, lattice orientation distribution, and plastic strain rate distribution are extracted from the simulation.

11:40 AM
Non Destructive Nanotomography Imaging in Structural Materials: *Henry Proudhon*[1]; Thilo Morgeneyer[1]; Erembert Nizery[1]; Lucien Laiarinandrasana[1]; Peter Cloetens[2]; [1]MINES ParisTech; [2]ESRF

Computed X-ray tomography has become routine to study many kind of materials at the micron scale. Third generation synchrotron and now X-ray lab sources allow in situ real time studies of the material behavior under all kind of solicitations. In both cases, classical setups works well typically up to 0.5 micrometer spatial resolution. To overcome this limitation, magnified holotomography has been developed at beamline ID16 (ESRF). An X-ray optics system focuses the synchrotron beam into a focal spot below 100 nm which is used a divergent source like in classical cone beam tomography. Two structural materials have been investigated using this setup: (i) a commercial aluminum alloy to determine the exact shape of second phase particles responsible for fatigue crack initiation and a deformed semi-crystalline high-density Polyethylene to determine the void population and gain some insight on the cavitation phenomenon.

12:00 PM
Scanning 3DXRD Technique using a Microbeam for In-situ Orientation and Stress Mapping: *Yujiro Hayashi*[1]; Yoshiki Seno[1]; Daigo Setoyama[1]; [1]Toyota Central R&D Labs., Inc.

A scanning-type technique of three-dimensional x-ray diffraction (3DXRD) microscopy is presented. In the scanning 3DXRD method, orientations and stresses in polycrystalline materials are mapped by means of an x-ray beam with the size of 1-2 \956m. The use of the microbeam is one of the solutions for the main problem with 3DXRD-based techniques, the overlap of diffraction spots from multiple grains on an area detector. Because of the use of not a near-field detector but a far-field detector, scanning 3DXRD provides spacious sample surroundings for a conventional in-situ stress tester like used in CT experiments. 3D data are acquired by the 3D sample scan consisting of one rotation scan axis and two translation scan axes. The in-situ 3D map with 37^3 voxels at the voxel size of 1^3-2^3 \956m^3 under stress is obtained by 33 Hz diffraction image data collection synchronized with the 20\176/s endless sample rotation.

12:20 PM Lunch

Advances in Reconstruction Algorithms: Use of Simulations and Forward Models in Data Reconstruction (Part 1)

Monday PM — Room: Salon III
July 11, 2016 — Location: Pheasant Run Resort

Session Chair: Charles Bouman, Purdue University

2:00 PM Invited
Thoughts About the Role of Forward Models in Microstructure Reconstructions: *Marc De Graef*[1]; [1]Carnegie Mellon University

Physics-based forward models of commonly used materials characterization modalities have the potential to substantially increase the reliability and accuracy of the resulting microstructure reconstructions. We will illustrate this concept by means of a numerical closed-loop validation experiment, in which we create a synthetic 3D microstructure, derive from it an EBSD data set through forward modeling, index the data set using a dictionary-based method, and then reconstruct the microstructure. A quantitative comparison between starting and resulting microstructures can then provide information about the accuracy of the reconstruction, as well as further insights into improved and, ultimately, optimized acquisition parameters (e.g., a more EBSD appropriate sampling grid step size) that would increase said accuracy. We will also illustrate recent advances in the integration of the EMsoft forward modeling package, in particular the EBSD component, with the DREAM.3D package.

2:30 PM
Improvements in Algorithms to Enable Real-Time Reconstruction of HEDM Data Using MIDAS: *Hemant Sharma*[1]; Jonathan Almer[1]; [1]Argonne National Laboratory

High Energy Diffraction Microscopy (HEDM) delivers in-situ microstructural information from the bulk of polycrystalline materials. This paper will describe the MIDAS-G package, developed at Advanced Photon Source (APS), for real-time reconstructions of HEDM data for both "near-field"(NF-) and "far-field"(FF-) HEDM. This is aimed towards providing feedback for the user, which can help drive the experiments and make the data reduction process more user-friendly. Using inexpensive GPU resouces, MIDAS can provide turnaround times of the order of minutes for both NF- and FF-HEDM. A number of optimizations to improve reconstruction quality for small-grained and deformed specimens will be shown. This work is supported by GE Aviation and AFRL.

2:50 PM
A Novel Reconstruction Method for 3D-EBSD Data Sets: *Peter Konijnenberg*[1]; Stefan Zaefferer[1]; Dierk Raabe[1]; [1]Max-Planck-Institute for Iron Research

Capacitive and thermal drift phenomena play an ever increasing role in the reconstruction and analysis of 3D EBSD data sets. Typically, drift manifests itself as an in-slice distortion, mainly perpendicular to the scan direction. On one hand, this leads to subtle in-slice distortions but on the other hand, also to considerable misalignments between neighboring slices. This anisotropy and the irregular temporal character of drift limit the success of methods based on a re-alignment of integral slices. We propose a novel approach to address the aforementioned issue. We utilize the anisotropy, by rearranging clusters of data points with a low degree of distortion (e.g. individual scan lines) within the total data set, until an optimum alignment is reached. The global minimum of the objective function is obtained by statistical means. Results will be discussed and evaluated at hand of a number of representative high-resolution data sets.

Advances in 3D Materials Modeling: Deformation Modeling with Experimental Validation (Part 1)

Monday PM — Room: Salon IV
July 11, 2016 — Location: Pheasant Run Resort

Session Chair: Akihisa Takeuchi, JASRI / SPring-8

2:00 PM Invited
Studying Slip System Activity in Deforming Crystals Using High-Energy X-ray Diffraction and Finite Element Crystal Plasticity Modeling: *Darren Pagan*[1]; [1]Lawrence Livermore National Lab

Heterogeneity of crystallographic slip has been associated with numerous failure mechanisms, including fatigue and fracture. The ability to measure crystallographic slip processes in-situ as a crystal plastically deforms is critical for the advancement of micromechanical models used to understand material failure. An overview of new experimental methods to quantify heterogeneity of slip (shear strains) from distributions of lattice plane orientation found using high energy X-ray diffraction will be presented. The utility of these methods will be shown with results measuring heterogeneity of slip in deforming single crystals in-situ. In addition, how these new experimental data can be combined with finite element crystal plasticity modeling to build a more complete picture of the development of heterogeneous slip in deforming crystals will be demonstrated. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

2:30 PM
In-Situ 3-D Characterization and Direct Micromechanical Modelling for Identification of Microstructure-Property Relationship in Polycrystalline Materials: *Ricardo Lebensohn*[1]; Pokharel Reeju[1]; Bjorn Clausen[1]; Cristina Garcia-Cardona[1]; Evan Lieberman[1]; Chris Chen[1]; Marian Anghel[1]; Timothy Ickes[1]; James Hunter[1]; David Rogers[1]; Robert Suter[2]; Anthony Rollett[2]; Paul Shade[3]; Darren Dale[4]; Jonathan Almer[5]; [1]Los Alamos National Laboratory; [2]Carnegie-Mellon University; [3]Wright-Patterson AFRL; [4]Cornell High Energy Synchrotron Source; [5]Advanced Photon Source

In-situ non-destructive 3-D characterization and micromechanical formulations that can use direct input and be validated by those emerging methods are enabling a deeper understanding of microstructural effects on mechanical behavior of polycrystalline materials. In this talk we report the synergistic combination of Fast Fourier Transform-based methods, which can efficiently use the voxelized microstructural images of heterogeneous materials as input to predict their micromechanical response, and High Energy Diffraction Microscopy (HEDM) and tomography obtained in single- and two-phase metallic aggregates that allowed us to study microstructure-property relationship in these materials with an unprecedented level of detail.

2:50 PM
Measurement of 3D Displacement Field from Few Tomographic Projections: *Clément Jailin*[1]; Thibault Taillandier-Thomas[1]; Martin Poncelet[1]; François Hild[1]; Stéphane Roux[1]; [1]Laboratoire de Mécanique et Technologie, ENS Cachan/CNRS-UMR 8535/Univ. Paris-Saclay

This paper aims at providing 3D volume images of a deformed specimen based on a full 3D image describing the reference state, obtained from conventional computed tomography and the 3D displacement field described by much fewer parameters than the specimen volume itself and determined from very few projections. This contrasts with standard "digital volume correlation" approaches that require the full reconstruction of the deformed volume. The reduction ratio in the number of projections (thus acquisition time) may be greater than 100 allowing for tracking motion at a fast rate (4D tomography). The displacement field is parameterized by the mesh nodal displacements determined from the minimization of the quadratic difference between computed projections of the deformed image and radiographs for selected orientations. To minimize the number of parameters, a regularization term based on the mechanical modeling of the displacement field with a linear elastic description is also considered.

Advances in Reconstruction Algorithms: Use of Simulations and Forward Models in Data Reconstruction (Part 2)

Monday PM — Room: Salon III
July 11, 2016 — Location: Pheasant Run Resort

Session Chair: Marc De Graef, Carnegie Mellon University

4:40 PM Invited
Dynamic Sampling and Reconstruction for Material Science: *Charles Bouman*[1]; [1]Purdue University

The traditional approach to imaging has been to design a sensor (i.e. imaging system) that can directly produce the best possible image quality. However, as the cost and complexity of designing imaging systems with low distortion, high resolution, and low noise increases, this traditional approach is becoming increasingly impractical. An alternative approach is to design and Integrated Imaging systems in which computation and sensing are tightly coupled in ways which can reduce cost and increase quality in the most demanding scientific imaging applications.In this talk, we present some new methods for dynamic image sampling and reconstruction, which can dramatically reduce acquisition time in SEM scanning of material samples by employing this Integrating Imaging approach. Our method is based on acquiring each new sample in a manner that maximizes the new information, and then uses this information to optimally reconstruction the required material cross-section using model-based techniques.

5:10 PM
Extracting the Magnetic Vector Potential of Magnetic Nanoparticles Using a Model Based Iterative Reconstruction Technique: *KC Prabhat*[1]; Marc De Graef[1]; Charles Bouman[2]; K. Aditya Mohan[2]; [1]Carnegie Mellon University; [2]Purdue University

Lorentz TEM observations of magnetic nanoparticles provide information on the magnetic and electrostatic potentials of the sample. These potentials can be extracted from the electron wave phase shift by separating electrostatic and magnetic phase shifts, followed by 3D tomographic reconstructions. Typically, tomographic reconstructions are performed by means of filtered back-projection (FBP) or simultaneous iterative reconstruction techniques (SIRT), which leads to reconstructions with significant edge artifacts. We propose a model-based iterative reconstruction (MBIR) algorithm to improve the reconstructed magnetic vector potential, $\mathbf{A}(\mathbf{r})$. In this method, we first reconstruct the electrostatic potential, V(r), which is a scalar quantity. Then we use the magnetic phase shifts acquired in two different tilt series in conjunction with the divergence-less condition to reconstruct all three components of $\mathbf{A}(\mathbf{r})$. Additional prior information such as influence of neighboring voxels is also incorporated for accurate reconstruction.

5:30 PM
Reconstructing 3D Polycrystalline Microstructure from Diffraction Contrast Tomography: *Harsh Narula*[1]; Jitesh Vasavada[1]; Hrishikesh Bale[2]; Christian Holzner[2]; Leah Lavery[2]; Sushil Mishra[1]; Asim Tewari[1]; [1]IIT Bombay; [2]Carl Zeiss X-ray Microscopy Inc.

Diffraction Contrast Tomography (DCT) is a new non-destructive 3D experimental technique which provides location of centroids, volumes and crystallographic orientations of the grains in a bulk polycrystalline material. In a nucleation growth process, it is possible to develop the final 3D polycrystalline microstructure through deterministic simulation. However, in general, the locations of grain nucleation are not the same as the grain centroids; hence, constructing a 3D grain microstructure from the information of grain centroids and their volumes is a non-trivial inverse problem. The present work studies the above inverse problem by modelling nucleation as a marked stochastic point process. The growth in this study is modelled as a Heaviside function of the marked variable with repeated Minkowski addition. The effect of neighborhood and marked variable has a strong influence on the geometric features of the final grain structure.

5:50 PM
Diffraction Intensity Simulations in Near-Field High Energy Diffraction Microscopy Reconstructions: *Robert Suter*[1]; David Menasche[1]; [1]Carnegie Mellon University

We describe the motivation for and the implementation of calculations of diffracted beam intensities appropriate for near-field High Energy Diffraction Microscopy (nf-HEDM). The calculations include relative intensity variations across the ~100 observed diffraction spots from each crystalline grain as well as geometry dominated variations within the spatially resolved spots. The standard set of factors are included: structure, atomic form, Debye-Waller, and a Lorentz factor that includes a cut-off of the usual divergence for scattering vectors near the rotation axis. We also include an "effective Debye-Waller factor" that accounts for defect induced atomic displacements within coherently scattering volumes. The model calculations are being developed through comparisons to data collected on a small gold wire sample. Generalizations of this work can compute non-Gaussian intensity distributions observed on far-field detectors (ff-HEDM) and thereby may lead to more precise estimates of elastic lattice strains.

Advances in 3D Materials Modeling: Deformation Modeling with Experimental Validation (Part 2)

Monday PM — Room: Salon IV
July 11, 2016 — Location: Pheasant Run Resort

Session Chair: Darren Pagan, Lawrence Livermore National Lab

4:40 PM Invited
High-Resolution X-Ray Computed Tomography at SPring-8 and Improvements of Imaging Properties: *Akihisa Takeuchi*[1]; Kentaro Uesugi[2]; Hiroyuki Toda[3]; Masakazu Kobayashi[4]; [1]JASRI / SPring-8; [2]Japan Synchrotron Radiation Research Insititute (JASRI)/SPring-8; [3]Kyushu University; [4]Toyohashi University of Technology

Several types of high-resolution x-ray computed tomographies (CT) by using x-ray microscope optics has been developed at SPring-8. The achieved spatial resolution is approximately 100 nm. For the purpose of quantitative and precise CT measurement, the optical system is severely required to attain a high linearity of image contrast and a large field of view, as well as the spatial resolution. In the present situation, a kind of optical off-axis effect called as a ringing shown as a strong periodic pattern noise is remarkable at the peripheral region of the field of view. In order to solve this problem, we have newly developed an x-ray optical device used as an x-ray objective lens. Details of the noise reduction by using this device will be presented. Present status of high-resolution x-ray CT systems at SPring-8 will be also shown.

5:10 PM
On the Origin of the Anisotropic Damage of X100 Line Pipe Steel using 3D in Situ synchroton-Radiation Tomography Investigation: *Yazid Madi*[1]; Juan Garcia[2]; Thilo Morgeneyer[2]; Henry Proudhon[2]; Jacques Besson[2]; [1]EPF-Ecole d'ingénieurs / Centre des Matériaux Mines ParisTech; [2]Centre des Matériaux MInes ParisTech

Line pipe materials have anisotropic mechanical properties, such as tensile strength, ductility and toughness. In this study, anisotropic ductility of an API grade X100 line pipe steel plate was investigated using in situ synchrotron-radiation computed tomography (SRCT) and finite element simulations (FEM). Unit cell calculations were used to show that this fracture behaviour is not related to plastic anisotropy. The origin of anisotropic rupture is then investigated on small axisymmetric notched tensile samples using SRCT at ESRF-Grenoble. Specimens were tested for loading along both plate rolling direction and long transverse direction ; tests were interrupted at various stages of deformation to perform scans.The in-situ data allowed quantifying both macroscopic deformation and microscopic damage parameters such as: porosity, void shape and void orientation. Nucleation at small particles aligned along the L direction was evidenced during plastic deformation. Coalescence of voids within clusters along L-direction clearly explained anisotropic rupture (coalescence in columns).

5:30 PM
Study of Residual Stress in a Ti-7Al Alloy: *Kamalika Chatterjee*[1]; Armand Beaudoin[1]; [1]University of Illinois at Urbana-Champaign

Finite element simulations are carried out to follow the evolution of residual stresses in Ti-7Al alloy, as developed through a process of combined bending and tension about a stress concentration. A virtual polycrystal geometry is generated using the position and orientation information of the grains. This information is obtained from High Energy X-Ray Diffraction (HEXD) experiments performed at the Advanced Photon Source of Argonne National Laboratory. A finite-element model using mesoscopic field dislocation mechanics (Roy et al., 2007) is employed to simulate the deformation history of bending, tension and unloading. Model predictions show good agreement with the experimental results generated from HEXD experiments. Conclusions from this work are that room temperature creep plays a role in the development of grain-level residual stresses, and grains deform mainly via prism slip.

5:50 PM
Prediction of Atomic Structure of Interfaces using Electron Microscopy and Atomistic Simulations: Fatih Sen[1]; Tadas Paulauskas[2]; Ce Sun[3]; *Eric Schwenker*[4]; Moon Kim[3]; Robert Klie[2]; Jianguo Wen[1]; Maria Chan[1]; [1]Argonne National Laboratory; [2]University of Illinois at Chicago; [3]University of Texas at Dallas; [4]Northwestern University

Solid-solid interfaces influence many exciting optoelectronic, mechanical, electrochemical, and piezoelectric properties of materials. Materials interfaces can be characterized by electron microscopy in two dimensions; however, three-dimensional atomic structure at the interface can be very difficult to determine, due to defects and disorder. In the present work, we aim to overcome this problem by combining atomistic modeling with electron microscopy image simulation and matching methods. We investigated interfaces in CdTe and CeO2 using STEM and predicted the 3D atomic structure using density functional theory and empirical interatomic potentials. We employed advanced global multi-objective algorithms to optimize the atomic structure with respect to match with STEM image and energetics. This work represents a step towards enabling the determination of 3D materials properties from electron microscopy for any system.

Poster Session

Monday PM
July 11, 2016

Room: Salon V&VI
Location: Pheasant Run Resort

P-1: 2-Dimensional Synchrotron Radiation Diffraction Measurement for 3-Dimensional Distribution of Strains with Sub-mm Spacial Resolution: *Hidehiko Kimura*[1]; Daigo Setoyama[1]; Satoshi Yamaguchi[1]; [1]Toyota Central R&D Labs., Inc.

Most of mechanical components have non-uniform residual stress gradient, which plays key roles in the fatigue process. For the reliability assessment, the measurement of the stresses in the internal as well as external locations is necessary. Synchrotron x-ray diffraction method suitable for crystalline materials requires a 2-dimensional detector for the measurement of a small volume with fewer grains. In this study, a novel technique to combine a 2D detector and specially fabricated slit system for 3-dimensional strain distribution measurement is introduced. The system consists of multiple rotating disks with spiral-shaped slits. This rotating slits system works in a similar manner as the double slits for conventional x-ray diffraction setup. The details and results will be shown in the talk. The synchrotron radiation experiments were performed at BL33XU (Toyota beamline) of SPring-8 with the approval of the Japan Synchrotron Radiation Research Institute (JASRI) (Proposal No. 2013A7012, 2013B7012, and 2014A7012).

P-2: 3-D Crystal Plasticity: Multi-Scale Simulation of Deformation Response in Metals: *Sriram Ganesan*[1]; Veera Sundararaghavan[1]; [1]Department of Aerospace Engineering, University of Michigan-Ann Arbor

A parallel 3D multiscale crystal plasticity finite element (CPFE) code has been developed as part of the integrated suite of computational tools for the DOE Software Innovation Center for Integrated Multi-Scale Modeling of Structural Metals. The code demonstrates parallel performance and scaling on large-scale problems with millions of degrees of freedom running on hundreds of processors. Using experimental microstructure images as input, the code has been used to compute, validate and understand response of crystalline aggregates to mechanical loading. The single crystal response in this code is based on rate independent crystal plasticity model and locally sensitive modified Predominant Twin Reorientation (PTR) scheme for twin system evolution. The poster will highlight the features of the code and the current work that is focused on validating the CPFE model by comparing with strain maps obtained from micro-scale digital image correlation (DIC).

P-3: 3-D Printing Emerging Technologies and Its Principles: Anurag Jha[1]; *Nirmal Singh*[1]; [1]ISM DHANBAD

3D Printing promises to produce complex biomedical devices according to computer design using patient-specific anatomical data. Since its initial use as pre-surgical visualization models and tooling molds, 3D Printing has slowly evolved to create one-of-a-kind devices, implants, scaffolds for tissue engineering, diagnostic platforms, and drug delivery systems. Fueled by the recent explosion in public interest and access to affordable printers, there is renewed interest to combine stem cells with custom 3D scaffolds for personalized regenerative medicine. Before 3D Printing can be used routinely for the regeneration of complex tissues (e.g. bone, cartilage, muscles, vessels, nerves in the craniomaxillofacial complex), and complex organs with intricate 3D microarchitecture, several technological limitations must be addressed. In this review, the major materials and technology advances within the last five years for each of the common 3D Printing technologies. The ability to design and fabricate complex, 3D biomedical devices is critical in tissue engineering.

P-4: 3-Dimensional Strain Distribution Measurement Inside Power Modules by Digital Image Correlation on Synchrotron X-Ray Laminography: *Hidehiko Kimura*[1]; Takashi Asada[1]; Satoshi Yamaguchi[1]; Takeshi Uyama[1]; Yujiro Hayashi[1]; [1]Toyota Central R&D Labs., Inc.

Power modules are one of the key components that influence the driving and environmental performance of electric/hybrid vehicles. The large current induces thermal strains inside the modules consisting of various materials such as metals and resin composites. Non-destructive measurement techniques are required to evaluate the internal strains and morphology for the reliability assessment. In this study, synchrotron x-ray laminography was conducted on power modules during thermal fatigue process. 3-dimensional distribution of the internal strains in the resin composites was obtained by digital image correlation method applied to the laminography images. The result shows large strain concentration at the internal corners. This technique enables the strain measurement of non-crystalline materials like resin composites. Combined with diffraction methods for crystalline materials, it will be a useful tool to develop high-performance power modules. The synchrotron radiation experiments were performed at BL33XU of SPring-8 with the approval of JASRI (Proposal No. 2014A7012 and 2014B7012).

P-5: 3D Characterization of Powder for Additive Manufacturing via Synchrotron X-Ray Microtomography: *Ross Cunningham*[1]; Anthony Rollett[1]; [1]Carnegie Mellon University

Direct Metal Additive Manufacturing is an emerging manufacturing technique that has been gaining significant exposure due to its potential ability to manufacture complex parts with shorter lead times, minimal post processing, and reduced material waste. Of this family of technologies, the powder-bed systems are some of the more developed. To date, a limited selection of powders has been available to machine users, but there is significant interest in expanding into a broader range of powders. However, in order to produce quality parts, these machines require powder that spreads properly across the powder bed. Additionally, factors like interior porosity can affect the behavior of final parts. Previous work has examined the rheological properties of a wide range of powders, but traditional characterization methods have been unable to adequately describe the differences between powders. This work uses synchrotron-based X-ray microtomography as a novel method to compare properties of metallic powders.

P-6: 3D Digital Representation of Knitted Textile Architectures: *Daniel Christe*[1]; Dani Liu[1]; Bahareh Shakibajahromi[2]; Chelsea Knittel[3]; David Breen[2]; Genevieve Dion[3]; Antonios Kontsos[1]; [1]Department of Mechanical Engineering and Mechanics,Drexel University; [2]College of Computing and Informatics; [3]Shima Seiki Haute Technology Laboratory, ExCITe Center, Drexel University

Smart textiles constitute an emerging class of architectured materials that can “see, hear, sense, and adapt”, envisioned as tailorable material platforms for wide-ranging applications. Knitted fabrics exhibit complex structure-property-performance relations. Compared to other structural materials, knitting gives the designer much finer control of the hierarchical material architecture. While knitting has become a digital fabrication method producing elaborate knitted structures from a broad array of input materials, the lack of predictive simulation capability hinders insertion of functional fabrics. The broader scope of this work is to develop physics-based simulation tools to study mechanical/multi-physics behavior. Here, we describe a scheme for constructing digital representations of textile architectures. We identify fundamental “building blocks” for several stitch types to generate 3D structures, based on designer data. These structures are then fed to computational mechanics codes to examine load transfer mechanisms, with the aim of establishing predictive structure-property-performance relationships to provide quantitative feedback to manufacturing.

P-7: 3D Grain Reconstruction Using Laboratory-based Diffraction Contrast Tomography: *Yubin Zhang*[1]; A. Lyckegaard[2]; P. Reischig[2]; C. Holzner[3]; E. Lauridsen[2]; [1]Technical University of Denmark; [2]Xnovo Technology ApS; [3]Carl Zeiss X-ray Microscopy, Inc.

In recent years, significant efforts have been made to develop 3D characterization techniques using high-energy synchrotron X-ray sources, e.g. diffraction contrast tomography (DCT). Very recently, the concept of synchrotron DCT was transferred to the laboratory and LabDCT™ is now available on the Zeiss Xradia 520 Versa x-ray microscope. At the moment, orientations, sizes and positions of grains in bulk samples can be obtained. However, 3D grain morphology information is not yet readily available. A new solution is proposed in the presented work by combining LabDCT with Ga enhanced microscopy to reconstruct the 3D grain structures of Al1050 samples. The reconstructed grain structure is compared in detail to that provided by the software of GrainMapper3D™ using mathematical tessellation. The power of the LabDCT technique and its potential application in materials sciences is demonstrated.

P-8: 3D In Situ Laminography and Digital Volume Correlation Study of Strain and Damage Interactions During Ductile Tearing: *Thilo Morgeneyer*[1]; Thibault Taillandier-Thomas[2]; Lukas Helfen[3]; Francois Hild[2]; [1]Mines ParisTech; [2]ENS Cachan/CNRS/PRES UniverSud Paris; [3]KIT

Strain and damage interactions during tearing of a ductile Al-alloy with high work hardening are assessed in situ and in 3D combining two recently developed experimental techniques, namely, synchrotron laminography and digital volume correlation. Laminography allows to assess regions of interest in large flat specimens. Digital volume correlation is based on the tracking of 3D laminography image contrast, which is caused by micrometer-sized internal voids and inclusions. Via simultaneous assessment of 3D strain and damage at a distance of 1-mm from a notch of a thin Compact Tension-like specimen, it is found that parallel crossing slant strain bands are active from the beginning of loading in a region where the crack will be slant (see Fig1). These bands have intermittent activity but are stable in space. One void is followed over the loading history and seen to grow and orient along the slant strain band at late stages of deformation.

P-9: 3D Virtual Heterogeneous Microstructure for Real Particulate Materials Modeling: *Yang Lu*[1]; Stephen Thomas[1]; [1]Boise State University

Existing concrete microstructural models of particles embedded in matrix materials are only represented by regular shape particles, i.e. spheres. However, the real particle shapes are more complex and sometimes play an essential role of macroscale properties. In this work, a real material model, Anm model, with irregular shape particles is proposed. The Anm model places multiple irregular shape particles into a pre-defined empty container according to the real parking density to build up a particles embedded in matrix material model. Employing the stochastic parking algorithm, parking accuracy, efficiency and density can be obtained by the following innovations: 1) a new contact function, extending overlap box (EOB); 2) the stochastic parking algorithm to associate a different aggregate shape database with each size bin, which is a promising application for broad particle-matrix composites; 3) an uniform thickness shell model put around each particle to model the interfacial transition zone (ITZ) effect.

P-10: 3D Visualization of Kirkendall Pore Formation and Evolution in Metallic Wires via In Situ Synchrotron X-ray Tomographic Microscopy: *Ashley Paz y Puente*[1]; Dinc Erdeniz[1]; Julie Fife[2]; Xianghui Xiao[3]; David Dunand[1]; [1]Northwestern University; [2]Paul Scherrer Institut; [3]Argonne National Laboratory

Traditionally, Kirkendall voids are undesirable as they often result in degraded mechanical, thermal, and electrical properties. However, the implementation of the Kirkendall effect as an alternative route to fabricate small-scale hollow structures has recently garnered attention due to the many benefits of this technique compared to more conventional methods. We demonstrate here that this concept can be used to convert 50 µm diameter titanized Ni wires and aluminized Ni-Cr wires into Ni-Ti and Ni-Cr-Al microtubes, respectively. Using a non-destructive 3D visualization technique is critical to investigating the Kirkendall pore formation and evolution in these systems. Therefore, to further understand the mechanisms involved in, and kinetics of, the pore evolution, in situ synchrotron X-ray tomographic microscopy experiments were conducted. Here we discuss the results of the tomography study and show that the combination of tomography and traditional ex situ metallography is a powerful approach to conduct diffusion studies.

P-11: 4D In-Situ Nanoscale Imaging of the Fracture Behavior of CMC Microcomposites: *Hrishikesh Bale*[1]; Marty Leibowitz[1]; Sergey Etchin[1]; Luke Hunter[1]; Benjamin Hornberger[1]; Leah Lavery[1]; Robert Ritchie[2]; Brian Cox[3]; David Marshall[3]; [1]Carl Zeiss X-ray Microscopy, Inc.; [2]University of California, Berkeley; [3]Teledyne Scientific Company Inc

We report on the development of a new in-situ mechanical load stage within nanoscale CT scanner used to subject a SiC ceramic matrix composite (CMC) sample to in-situ tensile loading and indentation to study the fracture behavior of the material. Due to its strong oxidation resistance and high strength, SiC is used in advanced structural applications, which demand consistent structural integrity under hostile service environments of temperature and mechanical loads over extended periods of time. To overcome its inherently brittle nature of failure, SiC is processed in the form of complex microstructural architectures derived by weaving bundles of fibers, including functional coatings on the fibers and incorporating several strategies to enhance the toughness of bulk composite. The results from the in-situ imaging experiment presented here, reveal for the first time, how cracks initiate and propagate in a CMC at the nanoscale thereby providing insight into the complex fracture behavior.

P-12: 4D In Situ Solidification of Nano-Composites With and Without Ultrasonic Treatment: *Rémi Daudin*[1]; Sofiane Terzi[2]; Pierre Lhuissier[1]; Marco Di Michiel[3]; Mario Scheel[3]; Elodie Boller[3]; Luc Salvo[1]; [1]Université Grenoble Alpes, SIMAP; [2]European Space Agency; [3]ESRF-The European Synchrotron

The appearance of new processing techniques using external fields, such as ultrasonic melt treatment (UST), allows producing new composites containing sub-micrometer ceramic particles by preventing their natural agglomeration in the melt. Processing such composites requires information on the interaction between the particles and the solidification front (engulfment or pushing). While ultrasonically assisted solidification of non-reinforced alloys is well documented, less is known about the impact of the dispersion of particles that can influence the dendrites growth mechanisms and hence the finale microstructure. Numerical simulations have shown that particles influence the dendrite morphology [1] but no experimental evidence on metals is reported. We present here experimental data obtained using 4D in situ fast synchrotron tomography (ESRF) showing the effect of UST on the solidification of Al-based nano-composites and more precisely on their impact on the dendrite morphologies during growth. References[1] L. Granasy et al., Nat Mater, 2 (2003) 92-96.

P-13: A 3D Phase-Field Model for the Simulation of L12 Ordered K-Carbide Precipitates in Low Density Steels: *Mahsa Rahnama*[1]; Alireza Rahnama[2]; [1]Isfahan University of Technology; [2]University of Warwick

A phenomenological stochastic phase field model of coherent precipitation of L1_2 k-carbide from a disordered FCC structure, and non-coherent precipitation of that from a disordered BCC structure in low density steels have been developed. It explicitly takes into account both the lattice misfit strain and the four types of antiphase domains formed as a result of the L1_2 ordering. Based on the concentration wave representation of the ordered state, a coarse grain approximation of the non-equilibrium free energy functional of concentration and long-range order parameters has been formulated. Its relation to the microscopic free energy model has been discussed. Precipitation kinetics and microstructural development of k-carbide in Fe-Mn-Al-C have been investigated by two and three dimensional computer simulations based on this model.

P-14: A Framework for Modeling Microstructural Characterization Errors and Their Effect on the Accuracy of Grain Ensemble Statistics: *Gregory Loughnane*[1]; Michael Uchic[2]; Michael Groeber[2]; [1]Mound Laser & Photonics Center, Inc.; [2]Air Force Research Laboratories

It is generally accepted that high spatial resolution experimental data with minimal noise is preferable for quantifying microstructural features and ensembles. However, blindly employing such logic towards three-dimensional mesoscale microstructural data collection often results in highly inefficient experimental measurements. One method to determine minimally-sufficient resolution sampling schemes and allowable noise levels is to model the observed sources of error and examine their effect(s) on the statistic(s) of interest. To this end, this study investigates the effect of two sources of error associated with serial sectioning experiments: voxel discretization of data, and the non-indexing of pixels within electron back-scatter diffraction maps. Equiaxed and elongated phantom reference microstructures were generated with high resolution and subsequently re-sampled, allowing both spatial resolution and noise to vary independently. Following the application of experimental cleanup algorithms, minimally-sufficient sampling schemes are provided, which are based upon user-defined settings for accuracy in the underlying microstructural distribution(s) of interest.

P-15: A Geometric Morphometric and Finite Element Approach to the Study of Juvenile Long Bones from Medieval Wharram Percy: *Sarah Stark*[1]; Simon Mays[2]; Jo Sofaer[1]; Sonia Zakrzewski[1]; [1]University of Southampton; [2]English Heritage

This paper evaluates juvenile development in long bones and their interaction in a biomechanical framework. This was neglected in the past due to the lack of accessible techniques to analyze bone shape, techniques that have now become available with the rise of geometric morphometrics and Finite Element Analysis (FEA). A dataset of femora (n=25), tibiae (n=31), and humeri (n=36) from 47 juveniles ranging from infancy to twelve years old, was collected from medieval Wharram Percy. Three-dimensional models were created by structured-light-scanning. Morphometric and FEA revealed there is a significant difference between age groups as shape development occurs in the metaphyses. The curvature in the midshaft becomes developed after age five, potentially reflecting an increase in loading patterns. By introducing morphometrics and FEA to osteology, and in specific developmental studies, size and shape can be teased apart and provide a more comprehensive understanding of bone growth and form.

P-16: A New Fast Simulation Tool for Optimized X-Ray Micro-Tomography Data Acquisition: *Barbara Fayard*[1]; Arthur Sonzogni[1]; Olivier Guiraud[1]; Pierre Latil[1]; [1]NOVITOM - Advanced 3D Imaging

X-ray tomography is a powerful non-destructive 3D imaging technique but acquisitions can be time consuming and expensive. In order to calculate the best experimental parameters and reduce the acquisition time while optimizing the data quality, Novitom has developed a new fast simulation tool for X-ray tomography. It is based on a mixed approach -ray-tracing and wave optics- for simulation involving a large variety of sources –synchrotron and laboratory-, detectors –CCD, CMOS, flat panel-, material descriptions and contrast modes -absorption, phase contrast, single distance phase estimation, dual energy ….- After a brief description of the physical and numerical approaches used to perform fast simulation of image formation in tomography, the presentation will focus on the comparison of the output results both with respect to more complete -but slower- Monte Carlo codes and with respect to experimental data acquired on phantom objects and challenging materials.

P-17: A New In-situ Far-Field High Energy Diffraction Microscopy Planar Biaxial Experiment: *Garrison Hommer*[1]; Jun-Sang Park[2]; Peter Collins[3]; Adam Pilchak[4]; Aaron Stebner[1]; [1]Colorado School of Mines; [2]Argonne National Laboratory; [3]Iowa State University; [4]Air Force Research Lab

Advanced structural alloys often possess complex microstructures and low symmetry crystal structures that exhibit twinning, phase transformation and variations in strength between families of slip systems. These attributes give rise to anisotropic and asymmetric mechanical behaviors. Because of this, their three-dimensional mechanical properties and mechanisms of deformation cannot be fully understood through uniaxial characterizations. To investigate these behaviors with multiaxial macroscopic loading, a custom planar biaxial load frame capable of in situ X-ray diffraction experimentation has been built. The instrument was designed to study any arbitrary plane-stress loading condition, in addition to load path change events. Thus, the micromechanics of full plane stress yield and transformation loci may be quantified in addition to path-dependent behaviors. We will review the new experimental capabilities and sample designs, as well as the first in-situ results toward understanding the micromechanics of biaxial cold-dwell fatigue failures in Ti-7Al.

P-18: A Potts Model Investigation of Complexion Transitions and Abnormal Grain Growth: *William Frazier*[1]; Gregory Rohrer[1]; Anthony Rollett[1]; [1]Carnegie Mellon University

The Potts Model of grain growth was adapted for the purpose of simulating abnormal grain growth (AGG) resulting from grain boundary complexion transitions. The transition in grain boundary structure between specific complexion types results in changes in properties. Where the transitions decrease energy and increase the mobility of boundaries, the influence of the processes causing these complexion transitions on the occurrence of AGG was explored. The influence of the processes on the fraction of transitioned boundaries given proximity to an abnormal grain was also explored. AGG occurred provided that such transitions are more likely to occur when adjacent to already transitioned boundaries. AGG was also found to occur provided that transitions were allowed after a predetermined amount of grain boundary motion. The simulations show how the AGG observed in certain ceramic systems can occur. Simulations and experimental analyses to discriminate the processes causing complexion transitions in such materials are discussed.

P-19: AI-Materials Science to Predict Stress-Strain Curve: *Yoshitaka Adachi*[1]; Sunao Sadamatsu[1]; [1]Kagoshima University

A combined technique of Bayesian inference and optimized artificial neural network (ANN) was applied to predict a stress-strain curve of a dual-phase steel using high-dimensional microstructural features which were acquired by a fully-automated serial section 3D optical microscope "Genus_3D". In addition, an instructed AI image processing technique was used to get appropriate image thresholding. AI materials science consisting of image acquisition, image processing, image analysis, and machine learning is considered as a potential tool for high-throughput materials development.

P-20: Approximate Method for Solving Freezing in Variable Property Porous Media: *Rahul Basu*[1]; [1]Sambhram Instt of Tech, VTU

The freezing problem in a 1D semi infinite medium, with coupled temperature and concentration is solved with variable diffusivity and conductivity. Integral techniques are applied to get the boundary layer for temperature and concentration and freezing velocities. Kirchoff's transformation for the dependent variable obtains and analytic solution for slowly varying parameters by a Goodman Energy integral method.Comparison between numerical and exact results is made in the case of one dimension. Very good agreement occurs low Stefan numbers , high conductivity and temperature ratios. The exponent in the integral formulation was not significant. Difficulties in extensions to capture the moving boundary in 2D and 3D are analysed with use of variable time steps and adaptive mesh methods. The approximate method extended to 2D and 3D is suggested with appropriate transforms and methods to reduce the number of variables, eg by transforming the 3D spherical to the 1 D rectilinear.

P-21: Automation of Grain and Phase Identification of Low Symmetry Phases for High Energy Diffraction Microscopy: *Branden Kappes*[1]; Andrew Petersen[1]; Harshad Paranjape[1]; Ashley Bucsek[1]; Aaron Stebner[1]; [1]Colorado School of Mines

High Energy X-ray Diffraction Microscopy (HEDM) provides 3D characterization of individual crystals within a polycrystalline volume, including orientation, grain shapes, and strain tensors. Correctly identifying crystals of individual phases from expansive 2D X-ray diffraction data sets is critical to the success of this technique. Currently, this process requires users "guess and check" threshold values, minimum spot size, initial lattice parameters and other analysis settings. As a result, reduction and manipulation of HEDM data sets are rarely achieved in real time. Furthermore, grain sizes and overlapping spots on area detectors currently prevent crystal identification of lower symmetry phases. We present a digitial image correlation algorithm to identify peaks of low symmetry and/or low symmetry phases from HEDM measurements. These are applied to a hexagonal magnesium alloy and to cubic + monoclinic 2-phase nickel-titanium shape memory alloys. We discuss their abilities, efficiencies, and potential for use in real-time data reduction and analysis.

P-22: Characterization of Graphite Morphology in Cast Iron by X-ray Computed Tomography: *Chih-Pin Chuang*[1]; Singh Dileep[1]; Peter Kenesei[1]; Jonathan Almer[1]; John Hryn[1]; [1]Argonne National Laboratory

It is well-known that the morphology of graphite plays a critical role in determining the physical and mechanical properties of cast irons. Current industrial standard to evaluate the morphology of graphite in cast iron relies mainly on the subjective comparison of 2D metallography images of the specimen and ASTM/ISO Standard images. However, what really matters is the 3D morphology of the graphite and its spatial arrangement within the alloy, which cannot be judged reliably from 2D slices. The development of high energy x-ray tomography in recent decades makes it a promising technique to characterize graphite morphology in 3D. In this study, we used x-ray tomography technique to perform 3D-characterization of graphite morphologies in different types of cast irons. The size, shape, spatial connectivity and structure of different graphite morphologies were examined in detail. In addition, the result of 3D analysis is compared with the traditional 2D technique.

P-23: Characterizing Grain Boundary Networks in 3D through Algebraic Topology: *Brian Lin*[1]; Gregory Rohrer[2]; Anthony Rollett[2]; [1]National Institute of Standards and Technology; [2]Carnegie Mellon University

The grain boundary network of a microstructure has traditionally been characterized by the fraction of different types of boundaries and triple junctions. However, these characterization methods are not a direct measurement of the grain boundary network itself. In this work we present the use of topology metrics to assess the connectivity of the grain boundary network. The inverse connectivity, determined by the ratio of the Betti numbers, is proposed as a metric for how different types of grain boundaries are connected. The Betti numbers are calculated by computational homology and treating the different microstructural features as cubical sets via an open-source program known as CHomP. The variations in the inverse connectivity are measured as function of the grain boundary disorientation in a synthetic generated 3D microstructure and compared to real FCC Ni microstructure, which exhibits differences in connectivity as certain types of boundaries are eliminated from the grain boundary network.

P-24: Classification of 3D Reinforcement Fillers using Neural Networks and Genetic Algorithms from TEM Images: *Roberto Fernandez Martinez*[1]; Maider Iturrondobeitia[1]; Julen Ibarretxe[1]; Pello Jimbert[1]; [1]University of the Basque Country, UPV/EHU

The process of classifying 3D nano-reinforcement fillers, which define the structure of the material, according to their shape using electronic microscope images is a complicated task, but the result of the classification can define the final mechanical properties of the material. This classification can be performed using variables that identify the object by its 2D shape. Neural networks technique is used to classify the aggregates using a methodology that tune parameters within the algorithm to improve the models performance. Also, and like the number of features is high to get accurate results, genetic algorithms are applied to make a feature selection in order to get robust and accurate models. Using feed-forward neural networks with a single hidden layer without feature selection, it is obtained an accurate 74.80% of positive classification, and using genetic algorithm to optimize the models the results are improved, obtaining a total accuracy of 75.75%.

P-25: Comparison of the Mechanical Properties of Crumpled Foils and Entangled Monofilaments: *Justine Papillon*[1]; Eric Maire[1]; Olivier Ondel[2]; Damien Fabrègue[1]; Michel Pérez[1]; [1]INSA de Lyon; [2]Université Lyon

Crumpled foils and entangled monofilaments are new types of architectured materials which exhibit interesting mechanical properties associated with a low price and an easily shaping process. The structure of these entanglements is complex and 3 dimensional in nature. Consequently, a precise experimental characterization is then difficult to achieve. X ray computed tomography however, proved to be very efficient for performing this characterization. In the present study, samples were submitted to in-situ compressive tests using X-ray tomography which enabled a 3D microstructural characterization of the complex architecture of these materials. The compression tests were performed with the sample being constrained inside a cylindrical die. Mechanical properties and internal complex mesostructures were investigated using this non-destructive technique in order to link the microstructure to mechanical properties. Moreover, numerical modelings was used in order to determinate the mechanical properties of this material and a good agreement was found with the experimental results.

P-26: Data Assimilation for Phase-field Simulation using Ensemble Kalman Filter: *Kengo Sasaki*[1]; Akinori Yamanaka[1]; Shin-ichi Ito[2]; Hiromichi Nagao[2]; [1]Tokyo University of Agriculture and Technology; [2]Earthquake Research Institute, The University of Tokyo

The phase-field method is attracting much attention as a powerful method to simulate and analyze the microstructure evolution on the basis of the total free energy of materials. The method has been applied to simulate that various phenomena occur in various metals such as solidification, phase transformation and grain growth. However, likewise in other numerical simulations, unknown parameters and initial conditions that strongly influence the simulation results exist. Therefore, identifying suitable parameters and initial conditions is one of most critical issues to perform accurate phase-field simulations. Meanwhile, data assimilation, which enables to improve the simulation models through an effective estimation of model parameters from experimental data, has been paid attention. In this study, we apply the ensemble Kalman filter, which is one of the sequential Bayesian filters commonly used in data assimilation, to the phase-field simulation of austenite-to-ferrite transformation in Fe-C-Mn alloy in order to estimate the parameters accurately.

P-27: Deformation at Triple Junctions in the Absence of Three-Dimensional Connectivity: *Ying Chen*[1]; Mingjie Li[1]; [1]Rensselaer Polytechnic Institute

In order to establish structure-mechanical property relationships for polycrystalline materials, mechanical properties of individual grain boundaries and triple junctions need to be determined. The current understanding of how strain in three adjacent grains is accommodated at a triple junction is very limited. It is also rather challenging to extract properties of individual grain boundaries and triple junctions in polycrystalline materials because it is difficult to separate their effects from three-dimensional grain constraint and three-dimensional connectivity effects. We instead use a bottom-up approach. We design tensile testing specimens with columnar grain structures and examine deformation in triple junction regions. In the absence of three-dimensional grain constraint, the observed deformation and mapped strain can be attributed entirely to the grain boundary or triple junction being studied. The fundamental understanding gained will be critical for establishing quantitative structure-property relationships of polycrystalline materials and will be useful for understanding three-dimensional measurements.

P-28: Determination of Materials Parameters by Combined 4D Experiments and Phase-Field Simulations: *Jin Zhang*[1]; Stefan Poulsen[2]; Peter Voorhees[2]; Henning Poulsen[1]; [1]Technical University of Denmark; [2]Northwestern University

We propose a novel method to determine materials parameters by direct comparison between 4D experiments and phase-field simulations. Material microstructural evolution is measured using in situ X-ray tomographic microscopy. Using the first frame from the experiment as initial conditions, microstructural evolution is simulated using the phase-field model. An iterative optimization technique is then used to find the material parameters that yield the best global match between the simulated microstructure and later frames from the experiment. The proposed method is applied to a hypo-eutectic solid/liquid Al-Cu system undergoing coarsening to determine the liquid diffusion coefficient.

P-29: Effect of Build Direction and Heat Treatment on Mechanical Behavior of IN 718 Fabricated by Selective Laser Melting: *Yen-Ling Kuo*[1]; Shota Horikawa[1]; Koji Kakehi[1]; [1]Tokyo Metropolitan University

Effects of build direction and heat treatment on mechanical properties of IN718 fabricated by selective laser melting (SLM) were examined at a room temperature and 650°C. The dendrite and the coarse columnar grains grew up along the build direction in the as-built material. The specimens were cut along the vertical and horizontal directions of as-built block. As-built specimen and STA (solution-treated and aged) specimen were prepared. The tensile strengths of STA specimens were higher than those of conventional cast and wrought (C&W) material both at the room temperature and 650°C because of the high-density of dislocations and fine precipitates which would be induced during the SLM process. The STA specimen showed isotropic tensile properties at the room temperatures; however, at 650°C, the horizontal direction specimen exhibited one fourth ductility compared to the vertical direction specimen because of inhomogeneous-size-grain distribution and elongated columnar grains with a very high aspect ratio.

P-30: Effect of Neutron Irradiation to Tensile Behavior in Fe-9Cr Alloy—A Study using 3D X-Ray Diffraction Microscopy: *Xuan Zhang*[1]; Chi Xu[2]; Jun-Sang Park[1]; Hemant Sharma[1]; Jonathan Almer[1]; Meimei Li[1]; [1]Argonne National Lab; [2]University of Florida

Developing advanced structural materials for nuclear reactor applications requires a deep understanding of microstructure-property relationship. In this study, we use far-field high-energy X-ray diffraction microscopy (FF-HEDM) to probe the microstructural changes in neutron-irradiated and unirradiated Fe-9Cr alloy before and after tensile deformation at the Advanced Photon Source at Argonne National Laboratory. The 3D reconstructions reveal that the deformation introduces the formation of sub-grain structure in the orientation space and large variations in microstrain. The results also show that irradiation-induced defects modify the microstructural evolution under tensile deformation. In combination with in-situ straining with 2D wide-angle X-ray diffraction study, which provides information on dislocation kinetics and coherent scattering volume change, a better understanding of the fundamental deformation mechanisms in an irradiated Fe-9Cr alloy is achieved.

P-31: Electron Tomography and Spectroscopy of Advanced Transistor Architectures: *Andrew Herzing*[1]; [1]NIST

The computing power of modern semiconductor devices relies critically on ever smaller components. Advanced transistor architectures in particular pose an extreme challenge for metrology as they are comprised of nanoscale features which are structurally and chemically complex. We have utilized electron tomography in the scanning transmission electron microscope in an effort to assess the three-dimensional structure and chemistry of such devices. This approach is quite powerful, however, the quantitative and even qualitative interpretation of features in the reconstructed volume is hampered by instrumental constraints and issues related to data quality and processing. These factors can be reduced by improved specimen preparation and data collection method as well as by employing advanced reconstruction algorithms.

P-32: Evaluation of Crystallographic Deformation Behavior in Aluminium Alloy by Means of Diffraction-Amalgamated Grain-Boundary Tracking (DAGT) Technique: *Kyosuke Hirayama*[1]; Hiroyuki Toda[2]; Kentaro Uesugi[3]; Akihisa Takeuchi[3]; [1]Kyushu University; [2]Kyushu university; [3]Japan Synchrotron Radiation Research Institute

We proposed new diffraction-amalgamated grain-boundary tracking (DAGT) technique, which was developed by combining the grain boundary tracking (GBT) technique and XRD using a pencil beam. The method provides a description of the crystallographic orientations of individual grains in polycrystalline material during deformation by 4D (3D + time). The main motivation of this study is to verify the plastic deformation behavior on the basis of DAGT technique.

P-33: Evolution of 3D Microstructure in Phase Transforming and Twinning Materials – A Novel Micromechanical Modeling and Synchrotron Diffraction Based Study: *Harshad Paranjape*[1]; Ashley Bucsek[1]; Darren Dale[2]; Joel Bernier[3]; Aaron Stebner[1]; [1]Colorado School of Mines; [2]Cornell University; [3]Lawrence Livermore National Laboratory

High-energy diffraction microscopy (HEDM) is a non-destructive diffraction data analysis technique that results in 3D reconstructions of grain-scale microstructure. However it is challenging to analyze fine microstructures with low-symmetry phases arising from phase transformation and twinning in certain advanced materials. Limited dynamic range of the detectors, size effects and limitations in objectively separating diffraction spots from two phases are the culprits. We present a forward modeling technique that uses micromechanical modeling predictions and simulated diffraction patterns to perform 3D reconstructions of such martensite microstructure. Preliminary results are presented on experiments performed at CHESS on single crystal NiTi. By applying this forward modeling technique, we identify which geometrically-related martensite modes are active and how the observed martensite microstructure compares to crystallographic predictions. This study uses NiTi shape memory alloys with monoclinic martensite as a model system, but the method can be applied to other phase transforming and twinning materials.

P-34: Extraction of Fiber Orientation in Composite Materials from 3D Micro-Tomography: *Barbara Fayard*[1]; Pierre Latil[1]; Arthur Sonzogni[1]; Olivier Guiraud[1]; Moreno Trlin[1]; [1]NOVITOM

X-ray micro-tomography can provide the microstructure descriptors required for the simulation of macroscopic behavior of composite materials. However, the image processing required to extract the descriptors from 3D reconstructed images is still non-straightforward for dense fibrous media. In this context, Novitom has developed a software suite for data processing of 3D images of fibrous materials. Several numerical approaches have been implemented for the measurement of fibers' orientation: 3D gradients, 3D oriented distance map, anisotropic Gaussians, mean intercept lengths and skeletonization. The performances –uncertainty, robustness, speed …- of each algorithm have been tested and compared on several representative model media: injected short fibers, fiber bundles mats and woven fabrics. To our knowledge, it is the first time that such a complete comparative study is performed. The benefits and limits of each numerical approach as well as strategies for data acquisition for the various fibrous media will be presented.

P-35: Finite Element Simulation of Damaged CFRP for Predicting Stiffness Degradation using 3D Stereology: *Chandrashekhar Hiremath*[1]; Swarnendu Bhattacharya[1]; Jigar Goda[1]; Anirban Guha[1]; Asim Tewari[1]; [1]IIT Bombay

Carbon fiber reinforced polymer (CFRP) composite undergoes various damage states as the structure is subjected to different loadings during the lifespan. As the amount of damage increases, stiffness of the structure decreases. In this study, a method is established to measure 3D microstructural damage and predict the stiffness degradation of a unidirectional CFRP. This is a true prediction since it relates the independently measured microstructure property (damage) to a mechanical property (stiffness). Experimentally, controlled damage in CFRP is created by cyclically loading the specimen at predefined stress ratio for different number of cycles. True 3D microstructural damage, as a function of number of stress cycles, is measured using quantitative stereology through optical microscopy. The results of optical microscopy are compared with 3D x-ray tomographic visualizations. Representative volume element (RVE) based finite element (FE) analysis is used to predict stiffness degradation and validate through experimentation.

P-36: Grain Boundary Curvature as a Function of Five Crystallographic Parameters: *Xiaoting Zhong*[1]; Gregory Rohrer[1]; [1]CMU

Both the populations and energies of grain boundaries have been measured as a function of the lattice misorientation and grain boundary plane orientation, the five crystallographic parameters. These techniques have been extended to measure grain boundary curvature as a function of the same parameters. To validate the new method and characterize the uncertainties that arise when curvatures are determined from discrete voxel-based data, ideal shapes (spheres and cubes) were examined at a range of resolutions. The main findings are that the accuracy of the curvature measurement depends on the resolution and the curvature of the object, with accuracy decreasing with lower resolution and higher curvature. The method was then applied experiment 3D microstructure maps containing 1000 to 3000 grains. It was found that grain boundary curvature is correlated to the grain boundary energy, with low energy, boundaries having low curvature, and inversely correlated to the grain boundary relative areas.

P-37: Grain Structure of an Irradiated Hafnium-Aluminum Metal Matrix Composite Material: *Donna Guillen*[1]; Zilong Hua[2]; Heng Ban[2]; [1]Idaho National Laboratory; [2]Utah State University

A thermal neutron absorbing material, comprised of 28.4 vol% HfAl3 in an aluminum matrix, was developed to serve as a conductively cooled thermal neutron filter to enable fast flux materials and fuels testing in a pressurized water reactor. Using the focused ion beam (FIB), a sample was fabricated to 25µm × 25µm × 20 µm and mounted on a grid. A series of operations were carried out repetitively on the sample top surface to prepare it for scanning electron microscopy (SEM). First, a 100 nm layer was removed by high voltage FIB milling. Then, several cleaning passes were performed on the newly exposed surface using low voltage FIB milling to improve the SEM image quality. Last, the surface was scanned by Electron Backscattering Diffraction (EBSD) to obtain the two-dimensional image. After 50 to 100 two-dimensional images were collected, the images were stacked to reconstruct a three-dimensional model using DREAM.3D software.

P-38: In-Situ Nano-Tomography at ID16B: The New Nano-Analysis Beamline at the ESRF: *Julie Villanova*[1]; Rémi Daudin[2]; Pierre Lhuissier[2]; Luc Salvo[2]; David Jauffrès[2]; Christophe Louis Martin[2]; Rémi Tucoulou[1]; [1]ESRF - The European synchrotron; [2]SIMaP university Grenoble Alpes

In the framework of the European Synchrotron Radiation Facility (ESRF) upgrade program, a new nano-analysis beamline has been recently built on ID16 port[1]. At 165m from the in-vacuum undulator source, ID16B endstation which offers a multimodal approach has been designed to accommodate several micro-analytical techniques (X-ray fluorescence, X-ray absorption, and X-ray diffraction) combined with 2D/3D X-ray imaging (XRI, such as magnified tomography and laminography). The beamline configuration offers an improved lateral resolution (40 nm), larger flexibility capable of in-situ experiments, and a monochromatic nanobeam tunable in a large energy range (6-65 kV). In this work, we present the different techniques available for 3D measurements at the beamline building on examples with high scientific and impact such as materials for new energy and nano-materials. We focus on ongoing developments with in-situ nano-tomography including high temperature experiments.[1] G. Martínez-Criado, J. Villanova, et al., J. Synchr. Radiat., 23 (2015), doi:10.1107/S1600577515019839

P-39: In Situ 3D Laminography Observation of Failure in Cast Iron Under Shear and Tensile Loading: Lutz Zybell[1]; Maik Horn[1]; Meinhard Kuna[1]; Lukas Helfen[2]; *Thilo Morgeneyer*[3]; [1]TU Bergakademie Freiberg; [2]KIT; [3]Mines ParisTech

Computed laminography has been introduced to synchrotron imaging set-ups to complement computed tomography for three-dimensional imaging of laterally extended (i. e. plate-like) specimens. The interest of the method is shown for non-destructive and in-situ measurements of regions of interest in large planar specimens where engineering-relevant boundary conditions have to be met. Here, in situ experiments with large flat shear specimens have been performed at ESRF. Nodular cast iron was studied during the entiredeformation process in a region of interest within the specimen. The mechanisms leading to ductile failure under shear loading such as shear band formation, void shape and void volume evolution are investigated in detail with micrometer resolution. Damage evolution for tensile loading was also assessed.

P-40: In Situ Dynamic Tomography and Its Applications in Material Science/Engineering at APS: *Xianghui Xiao*[1]; [1]Argonne National Laboratory

Dynamic tomography has been seeing rapid developments in technique and growth in applications in the recent years. It can track the morphological structure change in a dynamically evolving system in situ nondestructively. Compared to other in situ techniques, e.g. diffraction and spectroscopy, dynamic tomography has advantage of high temporal resolution and reasonable sensitivity. This presentation will introduce the current progress of dynamic tomography applications in material science and engineering at the dedicated tomography beamline 2-BM of the Advanced Photon Source. The challenges in dynamic tomography technique and applications will be discussed in these examples. A perspective of an ideal synchrotron beamline optimized for material science/engineering will be presented on the end.

P-41: In Situ Study of Elasticity, Plasticity and Phase Transformations in 301L Stainless Steel: *Jinesh Dahal*[1]; Harshad Paranjape[1]; Jun-Sang Park[2]; Hemant Sharma[2]; Darren Dale[3]; Joel Bernier[4]; Aaron Stebner[1]; [1]Colorado School Of Mines; [2]Argonne National Laboratory; [3]Cornell High Energy Synchrotron Source; [4]Lawrence Livermore National Laboratory

Traditionally, macroscopic anisotropy of mechanical behaviors and material microstructures have been studied independent of one another. Thus, there is little direct experimental evidence that correlates the existing microstruture with the macroscopic observation across multiple length scales. We have been working to fill the void by creating new non-destructive, far-field high-energy diffraction microscopy (HEDM) planar biaxial experiment. This capability enables us to define roles of deformation mechanisms within a bulk specimen in micron scale. Furthermore, the experiments are performed under multiaxial loading, which enables us to characterize of elastic and inelastic deformation in three dimensions. In this poster, we present the results of using this experiment to study the austenite-ferrite transformation in 301L Stainless Steel. Specifically, we are investigating the influence of granular boundary conditions and heterogeneous stress distributions, and to quantify the micromechanical interaction energies required to activate different transformation and slip mechanisms.

P-42: Investigation of Orientation Relationship and Growth Direction of Beta-Mn Phase in Austenite-Based Lightweight Steels Using 3D Microstructure Reconstruction: *Keunho Lee*[1]; Siwook Park[1]; Sang Sub Han[1]; Seong-Jun Park[2]; Kyu Hwan Oh[1]; Heung Nam Han[1]; [1]Seoul National University; [2]Korea Institute of Materials Science

Recently, many researches in steel industry have been focused on reducing the density of steel while maintaining high strength for automotive applications, leading to development of various lightweight steels with excellent specific strength and ductility. Among the lightweight steels, austenite-based steels based on the Fe-Al-Mn-C system show superior mechanical properties and weight reduction rates. After aging steps, micro/nano-scale precipitates are formed in such steel system. Among them, beta-Mn phase causes harmful effect on mechanical properties, inducing brittle fracture. However, there is a lack of research on precipitation characteristics of the beta-Mn. In this study, the orientation relationship and growth direction of beta-Mn was investigated by 3D microstructure reconstruction. The orientation relationship between the beta-Mn and austenite matrix was examined by combining electron backscatter diffraction and transmission electron microscopy. In order to identify a preferred growth direction of the beta-Mn, we carried out 3D serial sectioning utilizing focused ion beam tomography.

P-43: Large Volume 3D Characterization of Microstructures by Xe-Ion Plasma FIB: *Madeleine Kelly*[1]; Noel Nuhfer[1]; Gregory Rohrer[1]; [1]Carnegie Mellon University

Focused Ion Beam SEMs with orientation mapping capabilities using electron backscatter diffraction can be used to characterize three dimensional microstructures of polycrystalline materials. Because of the amount of time required to mill materials using conventional Ga-source FIBs, it was impractical to examine areas larger than 100 microns in lateral dimension. Newly available Xe-ion plasma FIB SEMs have greater currents and use a more massive ion, leading to milling rates as much as 50 times faster, making it practical to examine much larger volumes of material. For example, in less than three days, we measured 325 parallel orientation maps in Ti, each 220 microns by 60 microns; the milling time for each layer was about 2 min. Results for a variety of metals and ceramics (including Ni, Ti, and Al2O3) will be presented and the effects of volume on a variety of microstructural statistics will be discussed.

P-44: Mathematical Morphology Applied on the Development of Automatic Finite Element Meshing Tools in the Case of Biphases Heterogeneous Microstructures: *Franck N'Guyen*[1]; [1]ENSMP

In the theme of 3D microstructures biphasic mesh, we will, through the 3D image of a short fiber composite material, offer an exhaustive description of the image method to extract relevant morphological components that will be the basis of a surface triangulation. We give this triangular structure morphologically optimized as a basis for many of the input mesh commercial codes which uses as input source vector description of a 2D image or a surface triangulation of a 3D image. These meshing tools will be used in the context of a finite element calculation to evaluate the relevance of our morphological triangulation. The experimental basis of our study is the discrete representation of an image composed of voxels in 3D. This representation allows us to use mathematical morphology tools which by its topological or probabilistic concepts, allows direct application to the images when they are composed of two phases (ensemblist cases).

P-45: Methods for Determining Integral Mean Curvature of Grain Boundaries in 3D Reconstructed and Simulated Structures: Robert DeHoff[1]; David Rowenhorst[2]; *Burton Patterson*[1]; Catherine Sahi[1]; [1]University of Florida; [2]U.S. Naval Research Laboratory

The integral mean curvature of grain boundaries, Ms, is the key geometric term relating grain size and local boundary mean curvature to the rate of volume growth or shrinkage of individual grains. Three methods for measuring Ms have been developed by different authors over the past five years, with different theoretical and experimental approaches as well as different image processing requirements and most applicable structure, e.g., smoothed or voxelated. Two methods require full three-dimensional information about grain surfaces while one requires only identification of the 3D face or size class on a 2D examination plane. Recent comparisons of these techniques on the same images have shown fairly good comparison and similar sensitivity per effort expended. All are now automatable to allow higher numbers of measurements and improved sampling.

The availability of these multiple methods for measuring Ms will enable more rigorous examination of boundary curvature-based growth theories.

P-46: Microstructure Investigation of Long Period Stacking Ordered Structure Formation in Mg-Zn-Gd Alloys: *Satoru Yoshioka*[1]; Masahiro Ishida[1]; Tomokazu Yamamoto[1]; Kazuhiro Yasuda[1]; Syo Matsumura[1]; Shigeru Kimura[1]; [1]Kyushu University

Magnesium based alloys in Mg-Zn-Gd with long period stacking ordered (LPSO) structure have superior mechanical properties. The specific structure is formed by the aging procedure at high temperature (623 K <). Additionally, this system has many crystal structures depending on aging temperatures and holding times. In this study, our final goal is to investigate relations between morphologies and local structure around Zn and Gd on precipitation process of LPSO phase from Mg97Zn1Gd2 cast alloy. We adopt two analysis methods of scanning electron microscope equipped with focused ion beam (FIB-SEM) and x-ray absorption fine structure with using a micro-beam (micro-XAFS). The shapes of Zn K-edge x-ray absorption near edge structure (XANES) at the highly Zn concentrated regions are changed by aging. These changes of XANES spectrum are synchronized with the changes of 3D morphology observed by FIB-SEM.

P-47: Modeling Deformation Behavior of Two-Phase Titanium Alloys using Representative 3D Microstructures: *Sudipto Mandal*[1]; Anthony Rollett[1]; [1]Carnegie Mellon University

Beta-stabilized titanium alloys show significant changes in microstructure and strength due to variations in its thermomechanical processing. During deformation there is a substantial evolution in the texture in both alpha and beta phases, along with changes in the alpha morphology. All these factors are significant and elucidating their effects on properties will aid in the development and optimization of these materials. Representative 3D microstructures are created for two-phase titanium alloys with different morphologies of the alpha phase. The morphological change is presented as a justification for the flow softening phenomena observed in these alloys. An image based fast Fourier transform algorithm is used to model the deformation behavior of titanium alloys. Different stages of microstructural evolution during uniaxial compression are modeled by creating representative 3D microstructures with the alpha morphology varying from disk-like to globular. The responses are compared with experimental compression tests at different temperatures and strain rates.

P-48: Modeling of Anti-Corrosion Coatings from Combustion Slag: *Oleg Chizhko*[1]; [1]Foreign Department of Association for German Engineers

Mineral rest substances of the fuel from coal and from municipal solid waste are the inert contribution of the combustible nature resources, which does not take part in the burning processes and stay in form of liquid ash after exothermic gasification of energetic elements. These ballast compounds are treated with the thermal influence of inflammable matter and their structure transforms in correspondence with temperature conditions of existence for polymorphic modifications and with changeable content for additional components. There is the cause of technical synthesis of new complexes from oxides of the main geological unities. With aim of fabrication of anti-corrosion coatings, we expect the directed formation of aggregations for ionic constituents in molten state and the condensation of stable phases, characterized with closed packed symmetries.

P-49: Modeling of Localized Corrosion of Metals: *San-Qiang Shi*[1]; [1]The Hong Kong Polytechnic University

It is very challenging to model metal corrosion process such as pitting in 3D because of its multi-scale nature. This work develops a phase-field model to study metal corrosion. A system free energy density was proposed to solve the diffusion and phase field equations, and the Poisson's relation was used to govern the charge distribution and electrical potential distribution. At nanoscale, an electrical double layer across the metal-electrolyte interface was realized. The information was used in a larger scale simulation. The work plan is from 1D to 2D and eventually to 3D pitting corrosion modeling. Further developments are required to include the effect of corrosion products and mass/electron transports in solid phases. The work was supported by grant from Research Grants Council of Hong Kong (PolyU 152140/14E).

P-50: Modeling the Probability of Occurrence of Rarely Occurring Critical Microstructural Features: *Joseph Tucker*[1]; Tyler Weihing[2]; Michael Groeber[3]; Adam Pilchak[3]; [1]Exponent; [2]Southwestern Ohio Council for Higher Education; [3]Air Force Research Laboratory

Microtextured regions (MTRs, or macrozones) are aggregates of similarly oriented primary alpha grains and are deleterious to dwell fatigue properties of near-alpha titanium alloys. Analysis of multiple dwell fatigue crack initiation sites has revealed the presence of a critical microstructural neighborhood consisting of MTRs of two dominant orientations with respect to the applied stress. Due to the rare occurrence of such a configuration, and the cost associated with collecting large amounts of EBSD data, we propose a methodology to use large-scale synthetic microstructure generation to determine the probability of occurrence of these "weak links." High performance computing resources were leveraged to run DREAM.3D in an embarrassingly parallel mode to create thousands of cubic centimeters of digital material. The synthetic volumes were analyzed for the occurrence of critical features based on segmentation criteria from experimental characterization of minimum lifetime samples determining the number of critical microstructural neighborhoods per unit volume.

P-51: Morphological Analysis of γ' Shape Evolution in Single Crystal Nickel-Base Superalloys: *Ryan Harrison*[1]; Patrick Callahan[2]; Tresa Pollock[2]; Marc De Graef[1]; [1]Carnegie Mellon University; [2]University of California, Santa Barbara

γ' precipitates are of fundamental importance to the high temperature performance of nickel-base superalloys. They have a distinctive morphology originating from elastic stresses generated by the misfit between matrix and precipitate crystal lattices. Prior investigations of precipitate coarsening have revealed a progression of the particle shape with aging. Previous attempts to quantify these morphological changes have relied on shape descriptors that are only meaningful for the regular shapes present during the early stages of this evolution. In the present work, moment invariants are employed to quantify the shape of γ' precipitates during aging in single crystal ruthenium and rhenium containing nickel-base superalloys. Moment invariants of low orders (2nd to 4th order) have been used to quantify the precipitate shape evolution; we will present a principal component analysis of the moment invariants during the morphological evolution in an attempt to connect precipitate morphology with aging behavior.

P-52: Multiscale Characterization of Novel Copper-Carbon Materials: *Iwona Jasiuk*[1]; Sabrina Nilufar[1]; Gabriela Couvertier Santos[1]; [1]University of Illinois at Urbana-Champaign

We present results on multiscale characterization of novel metal-carbon materials, called covetics, in which metal and carbon are combined in a new way, beyond thermodynamic limit. Copper-based covetic materials, containing 0, 3, 5 and 9 weight percent carbon, were studied. We conducted tensile and compressive testing which gave Young's modulus, yield strength, shear strength, ultimate strength, and tensile elongation at failure and Rockwell and Brindel hardness tests. Nanoindentation measurements gave information on spatial distribution of local elastic moduli and hardness. In addition, we characterized the microstructure at different scales using scanning electron microscopy and transmision electron microscopy to obtain insights on grain size and form of carbon. The following enhancements in properties over the corresponding base materials were observed: higher strength, higher hardness (Rockwell, Vickers and nanoindentation), larger elongation, unusual deformation characteristics, and lower density. Thus, these materials show promise for wide range of engineering applications.

P-53: Non-Destructive Internal Lattice Strains Measurement using High Energy Synchrotron Radiation: *Jun-Sang Park*[1]; John Okasinski[1]; Jonathan Almer[1]; [1]Argonne National Laboratory

Diffraction technique using monochromatic x-ray has been widely used to measure the residual strains in engineering components. However, isolating a particular volume inside a large component and measuring the local residual strain is a challenge when monochromatic x-ray is used. In this talk, we describe a spiral slit system capable of isolating an interior volume in a polycrystalline sample and measuring the lattice strains in the volume non-destructively. We compare and contrast the spiral slit system and the conical slit system and experimental results obtained from using the two systems. The strain measurement results from several polycrystalline samples with non-cubic crystal symmetry are presented.

P-54: Novel Capabilities of Neutron Imaging at Pulsed Sources: *Markus Strobl*[1]; [1]ESS

Modern pulsed spallation neutron sources enable a new generation of neutron imaging instruments profiting from unprecedented brightness and intrinsic wavelength resolution capabilities. While this has little impact on conventional attenuation contrast imaging, it allows the efficient implementation of a range of novel modalities for 3D imaging of crystalline characteristics, magnetic structures and fields as well as small angle scattering characteristics of bulk samples and under various external conditions. First examples illustrate the potential to observe phase distributions or even individual grains in the bulk of applied engineering materials, the reconstruction of magnetic domains, spatially resolved quantification of structures beyond direct image resolution or magnetic vector field reconstructions. However, only the current advent of the first dedicated imaging beamlines will allow the full exploitation and development of these promising techniques and sophisticated instrumentation based on the unique features of neutrons as a probe for condensed matter research.

P-55: Correlation of Defect Structures and a Voxelized Representation of Powder Bed Fusion Process Conditions: *Michael Groeber*[1]; Sean Donegan[2]; Edwin Schwalbach[1]; Jonathan Miller; [1]AFRL; [2]BlueQuartz Software

There has been significant work to date in the metal powder bed fusion community focused on understanding the influence of global processing parameters on microstructure and defect content (e.g. beam speed, power,spot size). However, a range of other implicit details are important, though they are not necessarily simply described. The present work focuses on the development of a novel technique to assess the impact of the energy input process details on material quality. This requires transformation of both in-situ process monitoring data and build-intent information into a voxelized representation, subsequent fusion with post build x-ray CT measurements, and analysis to identify correlations between processing details and structure. An example case generated in laser powder bed fusion of Ti-6Al-4V demonstrates this process by identifying correlations between location specific processing details and porosity.

P-56: On the Use of Neural Networks to Train Denoising Filters for Tomographic Reconstruction of the Magnetic Vector Potential: *KC Prabhat*[1]; Marc De Graef[1]; [1]Carnegie Mellon University

A proper tomographic reconstruction becomes increasingly challenging when the number of projections is limited. The same is the case when projections are acquired through Lorentz TEM for the reconstruction of electromagnetic potentials of magnetic nanoparticle samples. Even the most advanced TEM holder, built specifically for the purpose of tomography, does not allow performing a full 180° tilt series. This leads to a poor reconstruction with noise and sample edge effects. For this reason, we propose use of a filter that depends on the acquired projection datasets to overcome the issues of limited tilt series. Neural Network (NN) approach is used to construct a data dependent filter. In particular, we will use the Aharonov-Bohm phase shift expression to generate a training dataset of electromagnetic phase shifts and subsequently, determine the weights for the filter. Then, we use the trained filters to enhance the accuracy of the tomographic reconstruction.

P-57: One Approach for an Out-of-ROI Reconstruction: *Valeriy Titarenko*[1]; [1]University of Manchester

In many cases a user tries to get the best resolution of a region of interest. Thus an axis of rotation is centered with respect of it and all projections are extended in some way in order to avoid ROI artefacts. However it may happen that for a given energy of x-rays a sample is too thick, so intensity of x-rays passed through the sample near this ROI tends to zero. Due to errors in input data reconstruction of the ROI as well as any other part of the sample becomes impossible. For this case we propose a method of replacing values for a central part of a sinogram assuming some known values of attenuation coefficients inside of the ROI. We still will not be able to reconstruct the ROI but the outer region can be restored.

P-58: OOF 3D: A Materials-Science Focused Finite Element System: *Andrew Reid*[1]; Stephen Langer[1]; [1]NIST

The OOF object-oriented finite element software, developed at the National Institute of Standards and Technology, provides an interactive FEM tool which packages sophisticated mathematical capabilities in a materials-friendly user interface. The program's workflow begins with real microstructural images, which can come from either microscopy or from simulations. Users then interactively construct finite-element meshes which match the material microstructure, on which they can then perform virtual experiments to examine structure-property relationships, including effective properties of the microstructure as a whole, examinations of the distribution of applied loads throughout the microstructure, and parametric studies of the variations of these quantities with changes in constitutive material parameters or boundary conditions. This talk will introduce the recently-released 3D version of this software, and will also describe the application interface which allows the software to be extended by users.

P-59: Optimization of Microstructure via 3D Image-Based Simulation: *Hiroyuki Toda*[1]; Han Li[1]; Dowon Seo[1]; Rafael Batres[2]; Osamu Kuwazuru[3]; [1]Kyushu University; [2]Tecnológico de Monterrey.; [3]Fukui University

The conventional materials development process involves design, evaluation and production, in that order. In the present study, microstructures are virtually optimized by means of an accurate image-based simulation (IBS) in which multi-scale 3D structures of materials, which are difficult even to quantify, are accurately reproduced. To render it a practical technique for microstructural control, usable in manufacturing, the representation of a given complex 3D microstructure is 'coarsened' to make it suitable to conventional materials design techniques. IBS is performed by modeling the microstructures of practical materials accurately in 3D. After the selection of an extremely limited number of kinds, morphologies and locations of microstructural features strongly affecting materials characteristics of interest, from an enormous array of microstructural features, the coarsening process thoroughly filters out a staggering amount of microstructural information. We perform the microstructural optimization of practical materials, as a demonstrator study, to prove the feasibility of the technique.

P-60: Optimization of Partially-Sintered Metal Powder Porous Materials for Transpiration Cooling: *Sébastien Pinson*[1]; Remy Dendievel[1]; Cécile Davoine[2]; Audrey Guyon[3]; [1]Grenoble INP; [2]ONERA-The French Aerospace; [3]Sintertech SAS

Transpiration cooling could be seen as a more air efficient cooling techniques for airplane engine hot parts. Replacing the current combustion chamber multi-perforated walls by porous ones could considerably increase internal heat transfers and lead to a substantial reduction of cooling air. For their ease of manufacturing, porous materials made of partially-sintered metal powders are potential candidates to compose these walls. Materials formed from spherical or irregular-shaped particles were analyzed. Flow and heat transfer simulations were performed on three-dimensional images of samples digitalized by X-ray tomography as well as on numerically created architectures. Effective thermal conductivities were assessed experimentally. The material geometrical parameters (porosity, specific surface area…) were assessed thanks to image processing. Relationships between material properties and these parameters were developed then implemented into a tool permitting the optimization of partially-sintered architectures achieving the desired cooling efficiency and minimizing the cooling air mass flow.

P-61: Porosity Analysis in Al-10Si-1Mg Components Additively Manufactured by Selective Laser Melting using Synchrotron X-Ray Computed Tomography: *Suraj Raghavendra Rao Krishna Rao*[1]; Ross Cunningham[1]; Tugce Ozturk[1]; Jaakko Suni[2]; Cagatay Yanar[2]; John Siemon[2]; Deborah Wihelmy[2]; Anthony Rollett[1]; [1]Carnegie Mellon University; [2]Alcoa

The defect content in additively manufactured Aluminum parts has been characterized. Three Al-10Si-1Mg parts were built with varying processing conditions through selective laser melting. Synchrotron-based high energy 3D X-Rays were used to perform computed tomography at the Argonne Photon Source facility. The tomographic data was reconstructed using TomoPy. Avizo 9 was used to characterize and analyze the three-dimensional imaging data sets. The three-dimensional characterization of the reconstructed data provided qualitative and quantitative results on the pore size, distribution and morphology. The three samples showed significant variation in the characteristics of pores. These characteristics strongly depended on the process parameters. The generation mechanism of these pores were investigated by linking the process parameters to the melt pool sizes.

P-62: Practical Considerations for Efficacy in Additive Manufacturing: *Vicki Barbur*[1]; Kenneth Sabo[1]; Michael Tims[1]; Daniel Widdis[1]; [1]Concurrent Technologies Corporation

Use of additive manufacturing is escalating; the expectation is it addresses metal part issues not only associated with 'just-in-time' needs, obsolescence, and remanufacture but also delivery of novel structures. Value-return is unknown due to concerns about parts validation, and existence of consistent processes. Design of experiment methodologies with an SLM machine investigate an 'operating window' for metal powders, including Inconel 625, identified critical process parameters and their impact on build quality and associated performance. Models generated demonstrating process integrity as well as an ability to simulate alternative conditions and accelerate future design/builds are included. Leveraging such to other metals, e.g., stainless steel, as well as ways to increase the knowledge base and positioning for parts acceptance will be discussed. We present a business assessment model, combining process methodology and material utilization to deliver a 'Total Cost of Part' in which geometry and surfaces impact viability of the Additive Manufacturing process.

P-63: Practical Issues with the Collection and Transfer of 3D Materials Data: *Sean Donegan*[1]; Mike Jackson[1]; [1]BlueQuartz Software

The collection and simulation of 3D materials data has revolutionized our understanding of properties and microstructure. As the field continues to expand, a large amount of focus is rightly placed on methods for analyzing and correlating this wealth of information. The development of new methods for analysis is ultimately spurred by collaboration; however, little effort is placed in ensuring the easy and scalable transfer of data. Additionally, as the size of materials data continues to expand, there is a growing need for establishing architectures for storing this data. We present several practical approaches, showcased by specific frameworks and file formats, for defining workflows and infrastructure that better enable communication and collaboration. The goal of these approaches is to speed the development of tools for analysis and knowledge discovery.

P-64: Present and Future of Neutron Imaging and Diffraction Techniques on Materials Science Beamline IMAT: *Genoveva Burca*[1]; W. Kockelmann[1]; J. Kelleher[1]; S. Kabra[1]; S.Y. Zhang[1]; J.A. James[2]; T. Minniti[1]; F. Montesino-Pousolz[1]; J.B. Nightingale[1]; E. Yang[3]; [1]STFC Rutherford Appleton Laboratory, ISIS Facility; [2]The Open University, Milton Keynes, UK; [3]STFC Rutherford Appleton Laboratory, SCD

In order to enhance the material analysis capabilities at the neutron spallation source, ISIS, UK and to complement the existing neutron analysis facilities, a 'cold' neutron imaging and diffraction facility for materials science, IMAT, was recently built at TS-2 ISIS, UK. IMAT will allow for spatially and energy-resolved neutron imaging and diffraction measurements. In addition to conventional 'white-beam' neutron radiography and tomography applications IMAT will offer energy-selective imaging for mapping microstructural properties down to a spatial resolution of 50 microns. IMAT will also offer residual strain analysis, phase analysis and texture analysis by neutron diffraction. IMAT will be able to combine neutron imaging and neutron diffraction techniques, to steer diffraction measurements by tomography driven diffraction technique (TDD) based on the SScanSS software. IMAT will be operated as a user facility formaterial science applications and is open for developments of time-of-flight imaging methods.

P-65: Production of Nanobridges with Controlled Diameter by Layer-by-Layer Assembly: Yingmeng Zhang[1]; Nicholas Kotov[1]; *Qing Zhu*[1]; [1]University of Michigan

Layer-by-layer (LBL) assembly usually has been used to achieve multilayer films. Here, a special polymeric nanopillar array on transparent plastic sheet was used as a three dimensional (3D) substrate. After superhydrophobic coating, these nanopillar arrays became superhydrophobic but still keeping transparent. Then LBL deposition was applied to the 3D superhydrophobic nanopillar arrays by dipping in PSS and PDDA solutions in a cyclic manner. The LBL assembly on the superhydrophobic 3D substrates is quite unusual. Instead of traditional growth of 2D multilayer films, uniform nanoscale bridges formed between the nanopillars, with parallel LBL nanobridges in the same direction. Furthermore, the diameters of the nanobridges are growing on a regular basis, when increasing LBL dip-coating cycles and the dipping-time. These small changes on structure can be reflected in the UV-Vis spectrum. Therefore, if we coat some thermal sensitive agent outside the nanobridges, it's promising to apply these nanopillar arrays to thermometers.

P-66: 3D Predictions of Additive Manufactured Microstructures using a Modified Potts Kinetic Monte Carlo Approach: *Jonathan Madison*[1]; T. Rodgers[1]; V. Tikare[1]; [1]Sandia National Laboratories

Metal additive manufacturing techniques can result in anisotropic microstructures with significant variability through a component. Giving rise to a dependence of material properties on not only traditional processing parameters (time, temperature, etc), but also the deposition and raster pattern used to in the build. Here, a modified Potts Kinetic Monte Carlo method will be presented which allows for the simulation of microstructure based on process inputs. The resulting microstructures are then analyzed to determine distributions of grain size and morphology. Here we will discuss implementing the method on complex, 3D domains and novel analyses used for interpretation and quantification of grain distributions and characteristics in 3D.Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

P-67: Quantitative Microstructure Analysis of Tungsten Heavy Alloy using Stereology: *Jitesh Vasavada*[1]; Saurabh Arvariya[2]; Sushil Mishra[1]; Asim Tewari[1]; [1]IIT Bombay; [2]General Motors India Pvt. Ltd.

Tungsten Heavy Alloy (WHA) is a material used in various space and other applications. This alloy system has a two-phase microstructure with a contiguous matrix dispersed with particles of tungsten. The property of the alloy is a strong function of the size, shape and contiguity of these tungsten particles. In this study detailed 3D quantification of the size, shape and contiguity of these tungsten particles is performed using classical stereology and through disector techniques. The measurements are assisted by AI algorithms for auto segmentation of tungsten particle contacts and are studied as a function of thermo-mechanical loading. Apart from the mean quantities, these measurements are further used to deconvolute the 3D size-orientation bivariate distribution of the tungsten-tungsten contacts. This provides an understanding of the spatial topology of the microstructure and the role it plays in the microstructure evolution during thermo-mechanical loading.

P-68: Ring Artefact Suppression by a 2D Image Filtering: *Valeriy Titarenko*[1]; [1]University of Manchester

Ring artefacts are usually the most pronounced ones which do not allow a user to get good quality segmentation for a reconstructed volume. Several methods based on analytical formula have already been developed. Unfortunately, these methods are designed to process only separate sinograms. A new approach uses similar assumptions as the original method but extends it to processing of sets of 2D projections. As a result for a given level of noise in input projections a user is provided with a procedure to construct a 2D filter which suppreses ring artefacts. The new method tends to show better quality of suppression compared to the original method and to preserve real features inside a volume.

P-69: Segmentation of Individual Fibres of Uni-Directional Composite from 3D X-Ray Computed Tomography Data: Kristine Jespersen[1]; *Monica Emerson*[1]; Anders Dahl[1]; Knut Conradsen[1]; Lars Mikkelsen[1]; [1]Technical University of Denmark

Compression strength of uni-directional (UD) composite materials is governed by the fibre misalignment together with the non-linearity of the matrix material. Performing compression test, a characterization of the fibre misalignment is therefore necessary. In the current study, 3D x-ray computed tomography (XCT) was performed on both glass and carbon UD fibre filament winded composites. From the scans the fibre centre lines were extracted using a dictionary based segmentation algorithm. The used segmentation algorithm was trained by initial manual segmentation, which makes it possible to segment individual fibre centre lines even for noisy data sets. From the segmented data, fibre misalignment was calculated and fibres were imported into the finite element software ABAQUS for further analysis. In addition, characteristic values describing the measured fiber misalignment was linked to experimental measured compression strength values.

P-70: Simulation of Controlling System of Shape Memory Nanotweezers: *Peter Lega*[1]; Victor Koledov[1]; [1]IRE RAS

Thermoelastic martensitic phase transition in Ni-Ti based shape memory alloys enables to create the micro- and nanotools controlled by small change in temperature (about 10 C). This makes it possible to create complex microrobotical systems of manipulation and treatment of various nanoobjects in nanoindustry, medicine, nanoelectronics etc. This work deals with the development of a physical and mathematical model of the micro manipulation system. System includes nanotweezers with shape memory effect on the basis of composite microactuator Ti2NiCu/Pt, located on the tip of tungsten needle. Control of nanotweezers is carried out by electric current heating, flowing through the micro diode, located on the needle. Micro diode provides both Joule heating and temperature measurement in order to close the feedback loop of the controlling system. The prototype of the controlling system was manufactured and tested. Simulation results are compared with results of preliminary experiments.

P-71: STEM-HAADF and Super-X™ XEDS Tomography of Complex Nano-scale Precipitates in High Entropy Alloys: Jacob Jensen[1]; *John Sosa*[1]; Daniel Huber[1]; Gopal Viswanathan[1]; Robert Williams[1]; Hamish Fraser[1]; [1]The Ohio State University

High entropy alloys are a relatively new class of materials garnering a great deal of attention due to their remarkable balance of properties, including high strength, toughness, and ductility. HEAs appear to offer new pathways to lightweighting in structural applications, however, to realize this potential requires considerable alloy development that will rely on integrated computational materials engineering. The development of accurate computational models to predict alloy performance requires a detailed knowledge of the morphology and interconnectedness of microstructural features. Due to spinodal decomposition, these alloys often consist of a mixture of nano-scale phases, and because of the compositional and structural complexity, it is desirable to characterize the morphology as well as the chemical nature of the precipitates. In order to gain a comprehensive understanding of the microstructure and obtain a novel perspective of 3D elemental segregation in AlMo0.5NbTa0.5TiZr, electron tomography using STEM-HAADF micrographs and super-X XEDS spectral images was utilized.

P-72: Stereological Constraints on Three-Point Correlation Functions: Jitesh Vasavada[1]; Sushil Mishra[1]; *Asim Tewari*[1]; [1]IIT Bombay

A microstructure can be described by the morphology and spatial statistics of its constituents such as voids, grains, phases etc. One way of quantifying these microstructural attributes is through intrinsic volumes and their distribution. However, an alternative approach to quantify microstructure is through correlation functions. These functions in general depict the microstructure through a set of abstract mathematical relations which, in limiting case approach specific mean intrinsic volumes of the system. For example, the limiting cases of a two-point correlation function leads to the knowledge of phase volume-fraction and interfacial area per unit volume. The present work derives the limiting behaviour of three-point correlation functions for two phase microstructures in order to establish their relationship with higher order morphological features.

P-73: Structural Reconstruction of Solidification Kinetics in Cast Iron with Spherical Graphite: *Simon Lekakh*[1]; [1]MST

A methodology of the structural reconstruction of solidification kinetic in cast iron with spherical graphite (SGI) is described. The methodology includes an automated SEM/EDX 2D analysis of micro-features in SGI structure and conversion to a 3D Population Density Function (PDFexp). A structure integrator was developed to simulate PDFsim for arbitrary nucleation and growth rates functions of the solidification time. Structure reconstruction in the real castings was done by inverse optimization and matching both PDF functions at unique parameters of graphite nodule nucleation and growth. It was shown that SGI solidification kinetics significantly differs from that predicted by basic nucleation models. Cooling rate and inoculation have large effects on the kinetics of graphite nodule nuclei formation during solidification. It was proved that observed bi-modal PDF function in well inoculated SGI is related to the second nucleation wave. Reconstructed solidification kinetics can help in industrial process optimization.

P-74: Synthetic Microstructure Realizations with Random Texture: Harsh Narula[1]; *Sushil Mishra*[1]; Asim Tewari[1]; [1]IIT Bombay

Crystallographic texture of metallic materials is a key microstructural feature, which governs their thermo-mechanical behavior. Current research work focuses on developing 3D synthetic microstructures having set of grains such that their crystallographic orientation is unbiased, which is also known as random texture. Mackenzie's algorithm is the most popular algorithm among the computational material scientists for generating random texture. However, its formulation involves square roots and may involve divisions with small numbers leading to computational inefficiencies as well as inaccuracies associated with floating point division. In this study two new algorithms are proposed to generate random textures. These essentially randomize the two axes of the unit cell in 3D to generate random texture. On comparison with Mackenzie's algorithm, these algorithms are more robust in terms of floating point calculations. Moreover, these new algorithms can be directly used to generate a large variety of constrained random textures (e.g. sheet and fiber texture).

P-75: Techniques for Advanced Image Processing and Effective Material Property Calculation for Microstructural Data: *Kerim Genc*[1]; Thomas Spirka[1]; Philippe Young[2]; Wojciech Smigaj[2]; [1]Simpleware Inc.; [2]Simpleware Ltd

Novel image-based techniques have been developed for processing, quantifying and calculating effective properties from 3D materials data (CT, micro-CT, SEM…). These techniques, implemented at Simpleware Ltd (Exeter, UK), enable materials data to be visualised, analysed and exported as models suitable for a wide range of design and materials applications. Particular advances have recently been made in image-based meshing from materials data, enabling very complex microstructure to be processed and converted into computational models.In addition, developments have been made in terms of calculating effective material properties such as stiffness, elasticity and permeability from materials samples using finite-element-based homogenisation techniques. These methods are applicable to areas such as composite research, oil and gas (analysis of core samples and reservoir characterization), and general materials science workflows involving materials data obtained from 3D scan modalities. This presentation will outline key elements of these workflows, with particular application to working with complex microstructures.

P-76: Three-Dimensional Microstructural Evaluation of Materials using Robo-Met.3D®: *Satya Ganti*[1]; Bryan Turner[1]; [1]UES Inc

Robo-Met.3D® is an automated metallographic serial sectioning system to probe the three-dimensional microstructure of materials. Automated serial sectioning allows for better regulation of slice thickness and surface preparation for more accurate 3D reconstruction. We report sequential image acquisition and processing details for the additively manufactured titanium alloy Ti 6Al 2Sn 4Zr 2Mo and ANSI 4130. Three dimensional reconstruction of the serially sectioned two-dimensional micrographs is then performed using open source and commercially available image processing software. This 3D analysis enables a direct measurement of features such as the pore size distribution in additively manufactured titanium alloy Ti 6Al 2Sn 4Zr 2Mo. The microstructural features of interest for the ANSI 4130 data pertain to the individual grains, grain boundaries, and phases present. Such analyses enable the three-dimensional visualization of microstructural features as well as the quantification of feature measurements and their correlation with material properties.

P-77: Three-Dimensional Nanostructure Determination Based on Scanning Electron Nanodiffraction: *Yifei Meng*[1]; Jian-Min Zuo[1]; [1]University of Illinois at Urbana-Champaign

We report on a high resolution and low-dose scanning electron nanodiffraction (SEND) technique for three dimensional (3D) nanostructure determination. A special sample holder is employed for a large angle rotation within a narrow polepiece gap. The 5-dimensional dataset, consisted of two diffraction coordinates, two projected sample coordinates and one rotation, is collected by performing SEND at various rotation angles. Acquired diffraction patterns (DPs) are then sorted and indexed for the grain orientation determination. The 3D morphology of a grain is reconstructed using an algebraic iterative algorithm under certain prior conditions. We demonstrate our technique using the nanocrystalline TiN thin-film as a test sample. The results show that this technique provides an effective and adaptive way to determine the grain morphology and orientation in nanocrystalline materials.

P-78: Understanding Transformational Faulting as a Deep Focus Earthquake Mechanism: Correlating In-Situ Acoustic Emission Locations at High Pressure and Temperature with Post-Mortem Fault Imaging Using Synchrotron X-Ray Microtomography: *Yanbin Wang*[1]; Feng Shi[1]; Lupei Zhu[2]; Tony Yu[1]; Mark Rivers[1]; Alexandra Schubnel[3]; Nadege Hilairet[4]; Fabrice Brunet[5]; [1]University of Chicago; [2]St. Louis University; [3]ENS-Paris; [4]Université Lille1; [5]Université de Grenoble

We studied transformational faulting from olivine to spinel in Mg_2GeO_4, an analog of the silicate olivine $(Mg,Fe)_2SiO_4$, using a high-pressure deformation apparatus in conjunction with in-situ acoustic emission (AE) monitoring. Synchrotron X-ray microtomography (XMT) was used to image the samples recovered from the deformation experiments, with spatial resolution of ~0.005 mm. We established spatial correlations between AE events observed during deformation and faults imaged by XMT post-mortem. A cross-correlation algorithm (hypoDD), developed for seismological studies, WAS adapted for locating the AE events, with a spatial resolution below 0.05 mm. This algorithm also helps separate events that share common characteristics in waveforms, which are likely related to different fault planes and faulting directions. These groups of events display excellent correlations with faults imaged by XMT, with two major groups of AE events correlating well with two conjugated faults in XMT images. These results help understand the dynamic process of transformational faulting.

P-79: Volumetric Elemental Imaging and Quantification by Confocal X-Ray Fluorescence: *James Mertens*[1]; Brian Patterson[1]; Nikolaus Cordes[1]; Kevin Henderson[1]; Jeffrey Griego[1]; Thomas Day[1]; Derek Schmidt[1]; George Havrilla[1]; [1]Los Alamos National Laboratory

Confocal Micro X-Ray Fluorescence (confocal MXRF) is a 3D spectroscopic technique capable of identifying constituents, measuring composition, and quantifying density variations in low density materials (~10 mg/cm^3). Confocal MXRF uses a polycapillary optic to focus x-rays from a source onto a sample. A second optic on the detector is used to detect x-rays only from the point of focus. Thus, it is possible to collect 3D MXRF data by point-by-point by step-scanning the sample. Previously we reported on a prototype instrument. Now, we've developed a new, second generation instrument which has resulted in improved scanning methods and enhanced transition metal detection. Design enhancements include: a higher power Mo tube; a vacuum chamber for enhanced detection of low energy x-rays characteristic of low *Z* elements; improved coupling of the optics to the detector; higher spatial resolution; and full spectral data acquisition. The instrument's capabilities will be demonstrated through thin film analyses.

P-80: Three-Dimensional Reconstruction, Visualization and Quantification of Dislocation Structures from STEM Stereo-Pairs: *Leonardo AGUDO JACOME*[1]; Kai Pöthkow[2]; Olaf Paetsch[2]; Hans-Christian Hege[2]; [1]Federal Institute for Materials Research and Testing (BAM); [2]Zuse Insitut Berlin

Dislocations, as carriers of plastic deformation, affect important properties in technical materials, e. g., plasticity. The realistic description of plastic deformation caused by dislocations demands the representative measurement of their features, e.g., line direction, slip plane, Burgers vector and density. Bulk deformation of structural and functional alloys requires reliable data from large regions. The filiform nature of dislocations interacting with complex microstructures additionally demands observation and analysis techniques that allow resolving the details of their interactions in space. The use of electron tomography for this purpose is bound to difficult and time consuming experimental setups, which are not always applicable to any material. In this contribution a new tool is presented, which enables the three-dimensional reconstruction, visualization and quantification of dislocation densities and directions from manual tracing of scanning transmission electron microscopy (STEM) stereo-pairs. Examples are shown from samples of a creep-deformed monocrystalline Ni-base superalloy.

P-81: Microstructure-Property Relationships in Metallic Castings: A Multi-Scale X-Ray Study: *James Mertens*[1]; Amy Clarke[1]; Brian Patterson[1]; Ricardo Lebensohn[1]; Kevin Henderson[1]; Damien Tourret[1]; Clarissa Yablinsky[1]; John Gibbs[1]; Seth Imhoff[1]; [1]Los Alamos National Laboratory

For complete process-to-performance predictions in castings, 3D microstructural modeling of both the solidification process and the mechanical response is required. Simulation validation relies on information obtained experimentally. Unfortunately, it is not possible to test samples that have been destructively imaged volumetrically; however, nondestructive techniques are available. Presently, we use x-ray micro-CT to volumetrically map solidification microstructures of varying composition in the Al-Cu system. Micro-CT spatial resolution and contrast is sufficient for imaging the eutectic and proeutectic phases. To resolve the eutectic lamellae, we use x-ray nano-CT. We compare CT results to solidification modeling predictions. To investigate the role of microstructure on the mechanical behavior of the castings, we implement in situ nano-radiography of micro-scale dogbone specimens. We correlate the measured mechanical response with the microstructure in the gage length, and we implement nano-CT and micro-CT to image the failure region. We also compare these results with micro-mechanical modeling predictions.

Plenary 2

Tuesday AM Room: Salons III&IV
July 12, 2016 Location: Pheasant Run Resort

8:00 AM Plenary
Revealing Microstructures using High-Energy X-rays: *Jonathan Almer*[1]; Peter Kenesei[1]; Jun-Sang Park[1]; Hemant Sharma[1]; Meimei Li[1]; Katherine Faber[2]; Stuart Stock[3]; [1]Argonne National Laboratory; [2]Caltech; [3]Northwestern University

High-energy x-rays from 3rd generation synchrotron sources, including the APS, possess a unique combination of high penetration power with high spatial, reciprocal space, and temporal resolution. These characteristics can be used to image microstructure with both traditional radiography and scattering modalities under a variety of environments. Over the past decade, the X-ray Science Division at the APS has developed specialized programs for these purposes, namely (i) absorption-based tomography, (ii) high-energy diffraction microscopy (HEDM), and (iii) combined small-and wide-angle x-ray scattering (SAXS/WAXS). Applications of these techniques to study several materials are presented. These include in situ studies- under thermal, mechanical and/or thermo-mechanical deformation - of high-temperature coatings, biological systems and nuclear-relevant materials. Specialized equipment to conduct these in-situ studies will be presented. Finally, opportunities to extend these capabilities through a proposed upgrade of the APS are discussed.

9:00 AM Break

Experimental Techniques for 3D Data Acquisition: Non-Destructive Methods for Investigation Material Response In-Situ

Tuesday AM Room: Salon III
July 12, 2016 Location: Pheasant Run Resort

Session Chairs: Ulrich Lienert, Deutsches Elektronen-Synchrotron; Michael Uchic, Air Force Research Laboratory

9:10 AM Invited
Single Grain High Resolution Reciprocal Space Mapping: *Ulrich Lienert*[1]; Wolfgang Pantleon[2]; [1]Deutsches Elektronen-Synchrotron; [2]Technical University of Denmark

Three-dimensional reciprocal space maps of individual grains within bulk samples have been recorded utilizing focused narrow bandwidth, high-energy synchrotron radiation and area detectors. Subgrain structure has been resolved in situ during tensile deformation of FCC metals. Fast time resolution is achieved since two dimensions are simultaneously covered by the area detector such that sample rotation is required only around a single axis. Key findings will be presented illustrating varying loading conditions. Experimental advances include the sole use of a single rotation axis for sample orientation facilitating the recording of several reflections per grain, a tension-compression capable load frame enabling fatigue loading, and the advent of efficient large area pixel detectors which will significantly accelerate data acquisition and improve reciprocal space resolution. The status will be reported and a novel experimental station which is being constructed at the PETRA III facility at DESY will be described.

9:40 AM
Using X-Ray Tomography to Study Damage under Load: Current Possibilities, Limits and Challenges: *Jean-Yves Buffiere*[1]; [1]Universite de Lyon INSA LYON

X ray micro-tomography is now an established characterisation technique increasingly used to obtain images of the interior of optically opaque materials with a spatial resolution in the micrometer range. Being a non destructive technique, it enables to monitor microstructure evolution during in situ experiments where, for example, some mechanical loading is applied.The aim of this presentation is to give an overview of the current possibilities of tomography to investigate in situ damage mechanisms in structural materials (cyclic or monotonic on metals or more brittle materials) but also, more importantly, to highlight the current limitations in order to suggest where further effort should be directed to. The presentation will make a comparison between synchrotron and laboratory experiments (which become more and more available) in terms of spatial and temporal resolution. Complementary experimental modalities (crystallography, quantification of strain …) will be illustrated as well as microstructural modelling (FEM, crystal plasticity...).

10:00 AM
Utilizing Non-Destructive Multimodal Experimental Techniques for 3D Characterization of Polycrystalline Materials: *Reeju Pokharel*[1]; Donald Brown[1]; Ricardo Lebensohn[1]; [1]Los Alamos National Laboratory

3D microstructural evolution in polycrystalline materials is characterized using high energy X-rays. The extremely high frequency and correspondingly low wavelength of the synchrotron X-rays enabled us to probe a range of materials with low to high Z-number. Diffraction and micro-tomography techniques were employed to study the microstructure evolution in polycrystalline Cu, during quasi-static loading condition. Also, microstructure evolution and effect of oxygen content in uranium fuel pellets has been probed at different thermal conditions to study the mechanics of grain growth and pore migration. Recent work has also been performed on additively manufactured stainless steel samples before and after heat treatment to monitor both as built and heat-treated microstructures. 3D data reconstruction and analysis to characterize polycrystalline materials under various material processes before, during, and after evolution in extreme environments are presented. The current analyses provide unprecedented data for the development and validation of microstructure based theoretical codes.

10:20 AM Break

10:40 AM
Probing Morphology and Chemistry in AISI 316 Stainless Steel using Correlative X-Ray and TEM Tomography: *Tim Burnett*[1]; Tom Slater[2]; R Bradley[2]; S Haigh[2]; P Withers[2]; [1]Manchester University/FEI; [2]University of Manchester

Here we present the first correlative tomography methodology study combining scanning transmission electron microscope (STEM) energy dispersive X-ray (EDX) tomography, focused ion beam (FIB) scanning electron microscope (SEM) imaging and nanoscale X-ray computed tomography (CT). This approach is applied to investigate the macroscopic location and distribution of nanoscale precipitates in a type 316 stainless steel by spatially correlating region of interest data from a STEM-EDX reconstruction to a precise location identified in a larger volume from nanoscale X-ray CT via intermediate SEM images. Investigation of a cavitated grain boundary reveals the three dimensional morphology of secondary phases of ferrite, M23C6 carbides and G-phase. The methodology outlined in this work extends the resolution limit for correlative tomography to the nanoscale. This approach could be extended to allow incorporation of data from other techniques, including atom probe tomography and electron energy loss spectroscopy.

11:00 AM
Multimodal X-ray Study of In-Situ Cracking in Titatium: *David Menasche*[1]; Paul Shade[2]; TJ Turner[2]; Ulrich Lienert[3]; Joel Bernier[4]; Darren Pagan[4]; Peter Kenesei[5]; Jun-Sang Park[5]; Robert Suter[1]; [1]Carnegie Mellon University; [2]Air Force Research Lab; [3]Deutsches Elektronen-Synchrotron; [4]Lawrence Livermore National Laboratory; [5]Argonne National Lab Advanced Photon Source

The development of nondestructive hard X-ray imaging techniques such as computed tomography (\956T) and far and near-field high energy diffraction microscopy (ff/nf-HEDM) has made possible in-situ characterization of damage development in bulk polycrystals. Here, we leverage these techniques to report on crack development in a commercial Ti7 alloy under uniaxial tension. After strain and orientation measurements were conducted using ff/nf-HEDM on the unstressed sample state, \956T was performed at various loading steps to interrogate the material density; when cracking was observed in the \956T reconstructions, more ff/nf-HEDM measurements were made to re-image the stress and orientation fields in the damaged region. Line-focused ff-HEDM was utilized to provide intragranular stress information and is combined with the fully spatially resolved orientation information from nf-HEDM. The effects of grain network morphology, crystallography, and stress development on crack nucleation and propagation will be discussed.

11:20 AM
Laboratory Diffraction Contrast Tomography – Applications and Future Directions: *Erik Lauridsen*[1]; Christian Holzner[2]; Florian Bachmann[1]; Kenneth Nielsen[1]; Leah Lavery[2]; William Harris[2]; Peter Reischig[1]; Allan Lyckegaard[1]; [1]Xnovo Technology ApS; [2]Carl Zeiss X-ray Microscopy, Inc

The introduction of diffraction contrast tomography as an additional imaging modality on the ZEISS Xradia Versa laboratory X-ray microscope has opened up a whole new range of possibilities for studies of the effect of 3D crystallography on materials performance. The non-destructive 3D crystallographic imaging capabilities of the laboratory diffraction contrast tomography technique (LabDCT), complements the structural data obtained by traditional absorption-based tomography and together they provide an unprecedented insight into materials structure.Here we will present a selection of results of LabDCT with particularly emphasis on its non-destructive operation, demonstrated through 4D evolutionary studies obtained by repeating the imaging procedure numerous times on the same sample. We will discuss the boundary conditions of the current implementation, and point to the future to discuss ways in which this can be correlatively coupled to related techniques for a better understanding of materials structure evolution in 3D.

11:40 AM
Diffraction Contrast in Neutron Imaging for Evaluation of Phase, Texture and Strain: *Robin Woracek*[1]; Dayakar Penumadu[2]; Anton Tremsin[3]; Nikolay Kardjilov[4]; Ingo Manke[4]; Markus Strobl[1]; [1]European Spallation Source; [2]University of Tennessee; [3]University of California at Berkeley; [4]Helmholtz Zentrum Berlin

Neutron imaging has experienced tremendous progress over the last decade, due to better detectors and by exploiting new contrast mechanisms, enabling phase contrast-, dark field , polarized neutron-, and neutron resonance absorption- imaging. Utilizing diffraction contrast offers the possibility to exploit the microstructure in the bulk (cm range) of crystalline materials in 2D and 3D. This presentation will outline the current status of transmission based neutron imaging at reactor and spallation sources. Emphasis will be given towards microstructural investigations using energy selective measurements that allow studying effects related to lattice strain, texture and crystallographic phase.The new pulsed neutron sources unlock another boost for neutron imaging. Ongoing method development includes full pattern refinement of transmission data as well as using additional detectors in diffraction geometry, paving the way towards 3D-neutron diffraction that is applicable to a broad variety of bulk samples.

12:00 PM
In Situ Characterization of Interaction and Coalescence of Stress Corrosion Cracks by X-Ray Microtomography and Digital Volume Correlation: *Thanh Tung Nguyen*[1]; José Bolivar[2]; Julien Rethore[3]; Marion Fregonese[2]; Jerome Adrien[2]; Jean-Yves Buffiere[2]; [1]LaMCoS INSA Lyon,CNRS; [2]MATEIS-INSA Lyon, CNRS; [3]LaMCoS INSA Lyon,CNRS

This project is aimed at characterizing and modelling initiation, interactions and coalescence of stress corrosion short cracks colonies by in-situ tensile tests performed in 3.5% NaCl solution on Al-Cu 2024 T3 alloy. The obtained results show that the microstructure presents a nice contrast between the aluminum matrix and Cu particles and that stress corrosion cracks colonies are obtained. The microtomography images are suitable for digital volume correlation (DVC). The noise measurement on the displacement field is about the usual value of about 0.1 voxel. Based on the measured displacement the strain fields have been computed from which crack initiation and propagation is tracked for. The formation of 3D micro-cracks is well captured. After the DVC analysis, the advected deformed image is also reconstructed which allows positioning the propagating micro-cracks onto the initial configuration. It emphasizes the role of Cu particles in the initiation of CSC for the analyzed material.

12:20 PM Lunch

Processing-Structure-Property Relationships in 3D: Microstructure Effects on Mechanical Response

Tuesday AM — Room: Salon IV
July 12, 2016 — Location: Pheasant Run Resort

Session Chairs: Jonathan Madison, Sandia National Laboratories; Michael Groeber, AFRL

9:10 AM Invited
Process-Structure Relationships in Metallurgical Joining and Their Implications to Mechanical Response: *Jonathan Madison*[1]; Olivia Underwood[1]; Lisa Deibler[1]; Jeff Rodelas[1]; Helena Jin[1]; Jay Foulk, III[1]; [1]Sandia National Laboratories

Metallurgical joining is a broad field including many processes and applications. In this work, laser-welds and explosive-bondings are examined for identification of defect populations as a function of their respective process parameters. Three-dimensional reconstruction and characterization of such defect fields allow for quantitative correlations to be made between processing and the resultant microstructure, while providing some insight to their mechanical responses observed in experiments. New insights gained through full-field three-dimensional understanding of the defect structure will be highlighted while detailing how such newly acquired understanding has either progressed knowledge of specific joinings or clarified previous misunderstandings or uncertainties in performance.Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000

9:40 AM
3D Mapping of Residual Stress Field in Shot-Peened Aluminum Alloy by Micro-Hole Drilling Method: *Bartlomiej Winiarski*[1]; Tim Burnett[2]; Matteo Benedetti[3]; Philip Withers[2]; [1]FEI & University of Manchester; [2]University of Manchester; [3]University of Trento

The complex 3D distribution and magnitude of residual stresses in aviation and aerospace components, particularly near stress concentrators, e.g. holes, notches, plays critical role in structural integrity and prolonging fatigue lifetime. Shot peening is frequently used to alter residual stresses because it can treat, with near-full coverage, geometrical details that are inaccessible to other surface treatments like ultrasonic peening or ball burnishing. The shallow treatment depth (some hundreds of microns) and the high lateral RS gradients (on the order of dozens MPa/μm) make many far-field experimental techniques unsuitable. In this work we introduce a combination of large volume serial sectioning by Xe+ Plasma FIB and micro-hole residual stress measurements. This has allowed us to map volumetric distribution of residual stresses in 3 dimensions and with a micron scale resolution. Here we present a first analysis of this approach applied to a shot peened 7075-T651 aerospace grade aluminium alloy.

10:00 AM
Effect of Microstructure on Tensile Behavior and Retained Austenite Stability of Thermo-Mechanically Processed Transformation-Induced Plasticity Steel Studied using In-Situ Synchrotron X-Ray Diffraction: *Elena Pereloma*[1]; Kun Yan[2]; Klaus-Dieter Liss[3]; [1]University of Wollongong; [2]University of Manchester; [3]Australian Nuclear Science and Technology Organisation

The austenite to martensitic transformation and phase strain evolution under uniaxial tensile loading of Fe-Mn-Si-C-Nb-Mo-Al Transformation Induced Plasticity steel subjected to different thermo-mechanical processing schedules were investigated using in situ synchrotron high-energy X-ray diffraction. The diffraction peaks from the martensite phase were separated from the peaks of the bcc matrix comprising polygonal ferrite and bainite. This allowed a more detailed analysis of lattice strains and load transfer between phases. The bcc matrix was shown to yield earlier than austenite and martensite. Some austenite grains start to transform at the stresses below that for the macroscopic yielding. The retained austenite in the sample with a lower fraction of ferrite (19%) transformed to martensite at a later stage compared with the sample containing a larger fraction of ferrite (30%) correlated to a finer microstructure and to a delayed work-hardening of the bcc matrix due to the higher volume fraction of bainitic ferrite.

10:20 AM Break

10:40 AM
Indentifying Fatigue Failure Sites in Rene 88DT via TriBeam Tomography: *William Lenthe*[1]; Jean-Charles Stinville[1]; McLean Echlin[1]; Tresa Pollock[1]; [1]University of California Santa Barbara

Fatigue is the life limiting property of polycrystalline nickel-base superalloys used for turbine disks. Identifying volumes amenable to crack nucleation and early crack propagation is a critical step in designing materials with improved fatigue life. A criterion for identifying fatigue crack initiating twin boundaries has been developed, with a strong dependence on elastic anisotropy. Volumes of the disk alloy Rene 88DT have been collected via TriBeam tomography at multiple resolutions to characterize microstructural features responsible for fatigue initiation. Calculation of the full elastic field for crack containing volumes verifies the initiation criterion. These 3D results are leveraged to enable extraction of initiation site statistics from 2D microstructures.

11:00 AM
Investigation of Nonmetallic Inclusion-Driven Failures: *Diwakar Naragani*[1]; Michael Sangid[1]; Paul Shade[2]; Jay Schuren[2]; Hemant Sharma[3]; Jun-Sang Park[3]; Peter Kenesei[3]; Joel Bernier[4]; Todd Turner[2]; [1]Purdue University; [2]Air Force Research Laboratory; [3]Argonne National Laboratory; [4]Lawrence Livermore National Laboratory

Crack initiation at inclusions is a dominant and unavoidable failure mechanism as fatigue progresses to find the 'weakest link' in the material to nucleate a crack. It is critical to identify a microstructurally informed driving force to characterize this failure mode. An experiment was conducted on a Ni-based superalloy sample with a seeded non-metallic inclusion under cyclic loading. The test was sequentially interrupted to conduct absorption contrast tomography to determine spatial and morphological information about the inclusion. Far field high energy x-ray diffraction microscopy was carried out to simultaneously characterize the microstructure. The centroid position, average orientation and stress state of the grains have been determined intermittently until crack initiation. The reconstructions elucidate temporal and spatial strain evolution of grains especially around the initiation site. Strain heterogeneity and the associated stress localization containing crucial information regarding damage evolution and accumulation are employed to determine the driving force for crack initiation.

11:20 AM
Investigation of Neighborhood Effects on Crack Initiation Sites in Different Ti Microstructures: *Vahid Tari*[1]; Michael Groeber[2]; Adam Pilchak[2]; Anthony Rollett[1]; [1]Carnegie Mellon University; [2]Air Force Research Laboratory (AFRL/RXCM)

Fatigue is a common and important failure mode in aerospace components. Many of these components are made of Titanium alloys because of their excellent mechanical properties. Their fatigue properties depend on the control of microstructure including grain size and morphology. To investigate the effect of varying the microstructure, we used a spectral full field elasto-viscoplastic method based on FFT to simulate the micro-mechanical response. A large number of three-dimensional synthetic input microstructures were generated based on experimental evidence. The results show that critical neighborhoods can be identified based on analysis of crack initiation sites.

11:40 AM
Intragranular Orientation Spread Induced by Grain Interaction: *Jette Oddershede*[1]; Grethe Winther[2]; [1]DTU Physics; [2]DTU Mechanical Engineering

Data on plastic deformation of metals monitored in-situ by three-dimensional X-ray diffraction microscopy (3DXRD) reveal that initially similarly oriented grains behave differently. The present focus is on two grains of near <522> orientation in the bulk of an interstitial-free steel subjected to 9% tensile deformation. The centre-of-mass orientations of the two grains neither rotate in the same direction nor with the same rate, and both develop internal orientation spreads of the order of 4 degrees. These differences originate from variations in the relative activities of the two most stressed slip systems, which are attributed to grain interaction effects. A spatially resolved map of the local environment of neighbouring grains as well as the orientation gradients within each grain has been reconstructed from the 3DXRD data. The grain interaction mechanisms are elucidated by crystal plasticity modelling based on the measured grain orientations and grain boundary planes.

12:00 PM
Constraint Effects on the Grain-scale Transformation Kinematics of Shape Memory Alloys Studied using High Energy Diffraction Microscopy: *Harshad Paranjape*[1]; Partha Paul[2]; Jun-Sang Park[3]; Hemant Sharma[3]; Aaron Stebner[1]; L. Catherine Brinson[2]; [1]Colorado School of Mines; [2]Northwestern University; [3]Argonne National Laboratory

We use high-energy diffraction microscopy (HEDM), a non-destructive diffraction technique for 3D reconstructions of hundreds to thousands of individual grains within a polycrystal, together with micromechanical modeling to study the kinematics of phase transformations in shape memory alloys (SMAs). Specifically, we document superelasticity (i.e., stress-induced phase transformation) in a polycrystalline SMA specimen by tracking the grain-scale strains, phases, orientations and volume evolutions during loading. We repeat the experiment after etching a surface layer of grains to expose some of the bulk grains. Through analysis of these data, we answer two key questions about the micromechanics of granular constraints on martensitic transformations: First, what is the effect of granular constraints on SMA performance? Second, how do the grains on the sample surface perform vs. grains in the interior? We also compare our HEDM measurements and conclusions with results obtained from digital image correlation (DIC) and micromechanical modeling.

12:20 PM Lunch

Experimental Techniques for 3D Data Acquisition: Improving the Efficiency and Accuracy of 3D Data Collection

Tuesday PM
July 12, 2016

Room: Salon III
Location: Pheasant Run Resort

Session Chair: Michael Groeber, AFRL

2:00 PM Invited
A New 3D Computational Method for 3D Orientation Data Sets for Uncovering the True Nature of the Deformed and Annealed States in Metals and Alloys: *Michael Ferry*[1]; [1]University of New South Wales

A major challenge in understanding structural changes during thermomechanical processing (TMP) of crystalline materials such as metals and alloys is the difficulty in viewing these generally complex structures in the most preferable case of three dimensions (3D). To address this 3D issue, there is an intense world-wide effort to develop a rigorous computational platform, applicable to any type of crystalline material, that can take a volume of experimental-derived orientation data and accurately reconstruct the microstructure in terms of its key features, including grains, grain boundaries, phases, interfaces etc. As part of this effort, we have developed a new boundary recognition method that substantially extends on a fast multiscale clustering (FMC) algorithm developed initially for feature recognition in conventional image analysis. Our modified FMC methodology is capable of automatically identifying the various types of low and high angle boundaries found in deformed and annealed metals using 3D orientation data sets such as 3D electron backscatter diffraction (3D EBSD). We will discuss the advantages of FMC for boundary reconstruction and why it is useful for understanding the origin of various structural features associated with TMP of a range of commercially-significant metals and alloys.

2:30 PM
Efficient 3D Characterization of Titanium Microstructures via Serial Sectioning Combined with Correlative Microscopy Methods: *Michael Uchic*[1]; Michael Groeber[1]; J. Michael Scott[2]; [1]Air Force Research Laboratory; [2]UES, Inc.

The 3D quantification of titanium alloy microstructures—especially at scales which are relevant for engineering applications—remains a technical challenge for the materials characterization community. Over the past five years, some of the present authors have conceived and developed a multi-modal characterization system that enables automated collection of electron-optic and light microscope data from metallographically-prepared samples that are approximately 30 mm in diameter. In this presentation, we highlight emerging pathways for efficient data collection for titanium alloys via the fusing and subsequent analysis of high spatial-resolution image data with electron backscatter diffraction maps collected at lower resolution. Examples of fusing both backscattered electron and optical images will be shown, for both model single-phase and two-phase engineering alloys that have been examined by the aforementioned automated characterization system.

2:50 PM
Comparison of 3D Pore Size Distribution using X-ray Computed Micro-Tomography and Serial Sectioning: *Amanda Levinson*[1]; David Rowenhorst[1]; [1]Naval Research Laboratory

Measurement precision of microstructural features is dependent on a number of variables including the measurement technique, resolution, and segmentation schemes applied. As there are multiple three-dimensional characterization techniques available, it is worth comparing their precision and efficiency. For this study, the pore size distribution in additively manufactured 316 stainless steel will be evaluated on the same volume using both x-ray computed micro-tomography on a Zeiss Versa 520 as well as serial sectioning coupled with optical microscopy. This will provide a one-to-one comparison of the void size distribution using both data collection techniques. The effect of resolution and segmentation will also be evaluated.

3:10 PM
Three-Dimensional Multimodal Imaging and Analysis of Ti–Ni–Sn Thermoelectric Materials: *McLean Echlin*[1]; Jason Douglas[1]; William Lenthe[1]; Ram Seshadri[1]; Tresa Pollock[1]; [1]UC Santa Barbara

Thermoelectric materials allow for the transformation of thermal gradients into voltages, which are interesting for capturing waste heat from energy production and transportation vehicles. The efficiency of these materials can be increased by engineering phonon scattering microstructures at a wide range of lengthscales thereby decreasing the thermal conductivity relative to the electrical conductivity. Femtosecond laser based tomographic data has been gathered using the TriBeam for Ti–Ni–Sn alloys with varying nickel content. The predominant phases present in the material, half-Heusler TiNiSn, and full-Heusler $TiNi_2Sn$ have a percolated structure, which changes as a function of alloying content. The very similar crystallographic structure of these phases requires multimodal data acquisition (EBSD, EDS) for the segmentation and reconstruction of both phases. The distribution and location of mesoscale phonon scattering sites, such as high angle boundaries have been measured quantitatively as well as coherent interface locations.

3:30 PM
Dictionary-Based Approach to Indexing of Electron Channeling Patterns: *Saransh Singh*[1]; Marc De Graef[1]; [1]Carnegie Mellon University

Electron Channeling Patterns (ECPs) were first observed nearly half a century ago and have been studied extensively in the literature. However, there is at present no general framework to automatically index ECPs. The Hough transform method, conventionally used in Electron Backscatter Diffraction (EBSD) indexing, is inadequate for ECPs due to the limited angular range of the patterns. In this contribution, we propose a forward model for ECP formation, and show that ECPs can be considered as zero-loss EBSD patterns due to the reciprocity theorem. We will show that the forward model, in conjunction with a novel dictionary-based approach, can be used as a robust and reliable indexing tool for this modality. We will compare observed and simulated channeling patterns for Austenitic stainless steel and compare the indexing results to those obtained from conventional EBSD analysis.

3:50 PM Break & Vendor Showcase

Processing-Structure-Property Relationships in 3D: Microstructure Effects on the Evolution of Materials

Tuesday PM
July 12, 2016

Room: Salon IV
Location: Pheasant Run Resort

Session Chairs: Burton Patterson, University of Florida; Dorte Jensen, DTU Risø

2:00 PM Invited
Analysis of Integral Mean Curvature Driven Grain Growth in Iron Using Diffraction-Contrast Tomography: Robert DeHoff[1]; Erik Lauridsen[2]; Dorte Juul Jensen[3]; *Burton Patterson*[1]; Yubin Zhang[3]; Catherine Sahi[1]; Christian Holzner[4]; [1]University of Florida; [2]Xnovo Technology; [3]Technical University of Denmark; [4]Carl Zeiss X-ray Microscopy, Inc.

Laboratory diffraction-contrast tomography (LabDCT) analysis has been used to obtain incremental time sequences of images throughout grain growth of polycrystalline Armco iron. These images allow measurement of curvature of grain faces, Ms, by face or volume class using the recent DeHoff technique. This method requires stereological counting measurements on 2D sections through 3D images in which the 2D grain sections being analyzed are identifiable by their above 3D property of volume or face class. This identification requires knowledge of the 3D structure of a sizable polycrystalline structure, obtainable only by serial section reconstruction or more directly and easily as done here by LabDCT analysis. These data have enabled a first-time experimental test of the DeHoff model of integral mean curvature driven grain growth predicting a linear dependence of dV/dt and Ms for grains of different groupings.

2:30 PM
Watching the Growth and Coarsening of Highly Anisotropic Alloys: *Ashwin Shahani*[1]; Xianghui Xiao[2]; Peter Voorhees[1]; [1]Northwestern University; [2]Argonne National Laboratory

Four-dimensional X-ray microtomography (4D-XRT) has made it possible to follow microstructural evolution in three dimensions and as a function of time. The advent of novel techniques in reconstruction, data processing, and visualization now opens the doors to a class of problems previously unexplored due to the lack of real-time 4D experiments. This is especially true of microstructures that have complex interfacial morphologies, such as group IV semiconductors. For instance, silicon and germanium exhibit “mixed” interfaces, i.e., partially faceted and partially rounded, due to the prevalence of defects that decorate the solid-liquid interfaces. Examples of our 4D-XRT results on the growth and coarsening morphologies of such structures, including the topological singularities that occur during microstructural evolution, will be given.

2:50 PM
Serial-Sectioning and Phase Field Models: Coarsening of Dendrites in Solid-Liquid Mixtures: *Thomas Cool*[1]; Peter Voorhees[1]; [1]Northwestern University

The morphological evolution of secondary dendrite arms during coarsening remains poorly understood. In particular, the mechanism governing the fissioning of secondary arms from the main dendrite stem remains controversial. We perform experiments on the International Space Station, since arms that fission from the stem do not sediment and thus can be detected. Once the samples were returned to earth, serial sectioning was used to create three-dimensional reconstructions, which can then be used to study the evolution of the microstructure. We measure both the morphology and topology (the genus) of the two-phase mixtures. We then also used the 3D reconstructions as initial conditions for a phase field method running on the GPU, allowing us to explore the time-dependent evolution of the structure. The results can then be compared to data taken at later coarsening times to provide insights into the processes controlling the evolution of these structures.

3:10 PM
Tracking 3D Microstructure Evolution during Powder Sintering by Laboratory X-Ray Diffraction Contrast Tomography: *Samuel McDonald*[1]; Peter Reischig[2]; Christian Holzner[3]; Erik Lauridsen[2]; Arno Merkle[3]; Michael Feser[3]; Philip Withers[1]; [1]University of Manchester; [2]Xnovo Technology ApS; [3]Carl Zeiss X-ray Microscopy

A new laboratory X-ray diffraction contrast tomography (LabDCT) modality has been used to follow the evolution of processes occurring during sintering of copper powder. In mapping the individual grains within the polycrystalline copper particles, non-destructively and in three-dimensions, the ability of the technique to track grain orientations and sizes over time is shown. Local diffusion and deformation-related shape changes of the sintering particles are captured using conventional absorption tomography. At the same time, LabDCT has enabled particle rearrangements (rotations and translations) to be inferred from measuring the changes in crystallographic orientation of grains. Such motions are important in contributing to the early stages of sintering together with associated development and growth of contacts between neighbouring particles. Over longer timescales, competitive grain growth from particle to particle has been tracked. The 4D study has given an improved understanding of the extent to which the different mechanisms contribute towards densification during sintering.

3:30 PM
***In-Situ* Multiscale 3D-Mapping of Embedded Recrystallizing Grains in Aluminium**: *Sonja Ahl*[1]; Hugh Simons[1]; Anders Clemen Jakobsen[1]; Dorte Juul Jensen[1]; Henning Friis Poulsen[1]; [1]Technical University of Denmark

Recrystallizing grains exhibit individual growth kinetics that depend strongly on the local lattice defects and their concomitant strain fields. Dark-field x-ray microscopy, a new synchrotron-based technique, enables 3D maps of the shape, orientation and strain of such grains with a spatial resolution of 100 nm and angular resolution of 5 µrad. In this work, we use in-situ high-speed reciprocal space mapping to track the global microstructural evolution during the recrystallization process. We then identify an individual grain of specific orientation and position and zoom in on the grain using dark-field x-ray microscopy to non-destructively map its internal orientation and strain in greater detail. Combining these techniques enables true *in-situ* multiscale 3D visualisation of both the boundary topology and the low density dislocation network inside recrystallizing grains. The results obtained for cold-rolled aluminium AA1050 show direct evidence correlating internal morphology and the shape and migration of the grain boundary during recrystallization.

3:50 PM Break & Vendor Showcase

4:50 PM
Characterizing Evolution in Commercial Li-Ion Batteries Across Space and Time using X-Ray, Light, and Scanning Electron Microscopy: *Jeff Gelb*[1]; Donal Finegan[2]; Paul Shearing[2]; Dan Brett[2]; [1]Carl Zeiss X-ray Microscopy; [2]University College London

With increasing dependence worldwide on portable solutions for energy storage, Li-ion batteries have seen a rapid increase in adoption. While these devices are now commonplace in many consumer applications, the mechanisms of both degradation and failure remain poorly understood. Here, we will show some recent results in using 3D microstructure-based characterization with correlative light, X-ray and scanning electron microscopy (LM, XRM, & SEM) to reveal the 3D morphology of the active layers within a commercial battery specimen. Furthermores, we will show how our recent work in characterizing the mesoscopic evolution of battery electrode assemblies using XRM relates to the capacity fade over the lifetime of a cell, providing new information about microstructure-based degradation & failure mechanisms.

5:10 PM
A Principle Curvature Analysis to Reveal the Isothermal Evolution of Nanoporous Gold: *Markus Ziehmer*[1]; Kaixiong Hu[1]; Ke Wang[2]; Erica Lilleodden[1]; [1]Helmholtz-Zentrum Geesthacht; [2]Technische Universität Hamburg-Harburg

Isothermal microstructural coarsening has always been of interest in material science, since, amongst others, it was recognized that microstructures can evolve in a self-similar manner. By way of example, the use of scaling laws is founded by the existence of such a self-similar evolution. Even though a structural characterization by one single metric is often sufficient, e.g. the (mean) grain or particle size, there are materials exhibiting a more complex situation with multiple salient structural features to be analyzed. One example is nanoporous gold, a system built up by interconnected ligaments that form irregular-shaped rings. In order to understand the coarsening of both components, we performed an analysis of the two surface principle curvatures on 3D reconstructed representative volumes of five samples. The use of marginal distributions showed that, strictly speaking, self-similar evolution cannot be stated. Moreover, it allowed for estimating the mean ligament and ring sizes.

5:30 PM
Three Dimensional Self-Organization during Three-Phase Eutectic Growth: *Abhik Choudhury*[1]; [1]Indian Institute of Science

Eutectic growth offers a number of examples of self-organization which are of interest both to materials scientists in terms of novel alloy development and for physicists in the context of an example of spontaneous pattern formation. While two-phase growth has been well investigated, in this regard, corresponding studies of three-phase growth are limited. In this paper, I will describe a numerical study using three-dimensional phase-field simulations to highlight the role of volume fractions of the solids in determining structure formation during directional solidification of three-phases in a ternary eutectic alloy. Thereafter, I will investigate the role of anisotropy in the solid-solid interfacial energy in determining morphological evolution and selection. As a final example, I will also show simulations of microstructural evolution using data of real alloys and highlight a comparison with experiments.

Processing-Structure-Property Relationships in 3D: Measurement and Understanding of Local Stresses and Nucleation Events

Tuesday PM — Room: Salon III
July 12, 2016 — Location: Pheasant Run Resort

Session Chair: Michael Ferry, University of New South Wales

4:50 PM
In Situ Characterization of Nanoscale Precipitate Nucleation and Growth in Aluminum Alloys Using Transmission X-Ray Microscopy (TXM): C. Shashank Kaira[1]; Sudhanshu Singh[1]; Vincent De Andrade[2]; Francesco De Carlo[2]; *Nikhilesh Chawla*[1]; [1]Arizona State University; [2]Advanced Photon Source, Argonne National Laboratory

Precipitation-strengthened alloys are ubiquitously used in almost all structural applications. Their superior mechanical performance can be attributed to the complex distribution, crystallography, and coherency of precipitates in the matrix. An accurate understanding of structure-property correlation in the alloy allows prediction of its deformation behavior, which is controlled by the morphology, size, shape and distribution of precipitates present. Conventional techniques like transmission electron microscopy and atom probe tomography fail to offer a 3D view of a statistically relevant region in the system. In situ

3D X-ray Tomography using Transmission X-ray Microscopy (TXM) has been utilized in this study to obtain a thorough representation of the microstructure present in aluminum alloys. Owing to its high spatial resolution, non-destructive nature and quick acquisition time, Transmission X-ray Microscopy (TXM) enabled not only ex situ analyses, but also, high temperature in-situ studies to understand and quantify the evolution of nanoscale precipitates in these alloys.

5:10 PM

Microstructural Effects on Void Nucleation in Polycrystalline Copper: *Evan Lieberman*[1]; Anthony Rollett[2]; Curt Bronkhorst[1]; Ricardo Lebensohn[1]; [1]Los Alamos National Laboratory; [2]Carnegie Mellon University

We present an investigation into the microstructural and micromechanical influences on ductile damage nucleation at polycrystalline grain boundaries. To achieve this aim, High-Energy Diffraction Microscopy (HEDM) measurements of a copper polycrystalline sample were made before and after a shock loading shock-loading experiment and the two data sets were used to establish the location within the pre-deformed sample of voids measured in the post-deformed sample. We then compare the occurrence of damage within the pre-deformed sample with micromechanical values obtained using a model with a Fast-Fourier Transform-based elasto-viscoplastic (EVPFFT) formulation. The model produces full-field solutions for the stress and strain in voxelized polycrystalline microstructures. In addition to standard micromechanical factors like stress and strain, we also consider morphological influence using surface normals calculated directly from the voxelized image using first order Cartesian moments. We compare distributions of these factors in the vicinity of the void locations with the overall distribution.

5:30 PM

Measured Resolved Shear Stresses on Slip Systems in Austenitic Steel Grains: *Nicolai Juul*[1]; Grethe Winther[1]; Jette Oddershede[1]; [1]Technical University of Denmark

A polycrystalline austenitic steel sample was subjected to a uniaxial tensile test while measuring the stress states of individual grains using three-dimensional X-ray diffraction (3DXRD). The resolved shear stresses (RSS) for grains with orientations within 10° of <100>, <110>, <111> and <321> were determined at strains of 0.1% and 1%. The RSS-values are compared to the calculated Schmid factors for uniaxial tension and the expected Bishop-Hill stress states, but differing somewhat from both of these. Some variations between grains of similar orientations are also observed, suggesting an effect of grain interactions. The differences will be correlated with the actual local environment of neighboring grains for each grain. The aim is to better understand the elasto-plastic transition of individual grains in polycrystalline aggregates.

5:50 PM

Quantitative 3D Mapping of Local Stresses Near Dislocation Channel-Grain Boundary Interaction Sites in Irradiated Stainless Steel: *Drew Johnson*[1]; Bryan Kuhr[2]; Diana Farkas[2]; Gary Was[1]; [1]University of Michigan; [2]Virginia Tech

The component of stress normal to the grain boundary near dislocation channel-grain boundary (DC-GB) intersection sites was determined using High Resolution Electron Backscatter Diffraction (HREBSD) and measurements of the grain boundary character in an irradiated austenitic stainless steel. Following straining in high temperature argon, strain maps were produced by measuring shifts in Kikuchi structure by cross correlating EBSD patterns. Strains were coupled with elasticity coefficients to calculate residual stresses. Subsequent straining in high temperature water induced Irradiation Assisted Stress Corrosion Cracking (IASCC). Plasma focused ion beam milling was used to determine the orientation of thousands of grain boundary planes, which were combined with EBSD data to fully determine the grain boundary character. Grain boundary normal stresses at DC-GB intersections could then be correlated to the occurrence of cracking. Coupled with molecular dynamics simulations of stress localization, these experiments provide the capability to determine the local stress required to initiate IASCC.

Advances in Reconstruction Algorithms: Interface Quantification and the Registry of Multi-Modal Data

Wednesday AM	Room: Salon III
July 13, 2016	Location: Pheasant Run Resort

Session Chair: Elizabeth Holm, Carnegie Mellon University

8:00 AM Invited

Accurate Reconstruction of Interface Geometries from Serial-Sectioning Data: *David Rowenhorst*[1]; [1]The US Naval Research Laboratory

During serial-sectioning, the need to accurately reconstruct geometry prefers a set of closely spaced sections while the need for collecting large statistical volumes within a reasonable time period requires that a large amount of volume be analyzed with as few sections as possible. The optimum solution is one where a high fidelity image is collected in each 2D section, and a larger spacing from section-to-section to collect large volumes. This then leads to a representation of the 3D structure made up of anisotropic voxels, and the interfaces take on a characteristic stair-stepped appearance. In this presentation we will discuss methods that have been developed to reduce these artifacts within reconstructions of serial-sectioned data, including corrections to slice alignment as well as surface-meshing constructions and smoothing techniques. Furthermore we will investigate the effects that these methods have on the measurement of key interfacial measurements including interface orientations and interface curvatures.

8:30 AM

Multi-Modal Fusion of Experimental and Simulated Materials Data: *Sean Donegan*[1]; Mike Groeber[2]; Mike Uchic[2]; Adam Pilchak[2]; Dennis Dimiduk[1]; [1]BlueQuartz Software; [2]Air Force Research Laboratory

As new characterization and simulation techniques are developed and utilized, materials data is becoming increasingly multi-modal. A key task when trying to analyze multi-modal data is the capability to fuse disparate kinds of data that are representative of the same component. Fusion may involve both affine and non-linear transformations of the underlying geometrical representations to enable co-registration of the data sets. These workflows are made more difficult when the data sets exist in different reference frames and scales, and are complicated by irregular geometries, such as meshes or CAD representations. We present several approaches for dealing with the fusion of multi-modal data, inspired by work within the image processing communities. The approaches are applied to several example experimental and simulated data sets. We also showcase the need for advances in fusion pipelines as new materials manufacturing processes are developed, especially within the scope of additive manufacturing.

8:50 AM

High Accuracy Heterogeneous CAD Against Tomography Registration: *Yann Le Guilloux*[1]; [1]Safran Paris-Saclay

Geometric registration between a tomographic image and a CAD-type model is a common prerequisite for most analysis tasks, at least in order to be able to locate indications with respect to a reference frame. A common approach involves first extracting a surface from the tomographic image, then matching it with the CAD model. Unfortunately, poor tomographic contrasts - as may arise in particular with concave parts - produce inaccurate surfaces, which in turn degrade the quality of registration. Our analysis concludes that deciding where the surface lies happens too early in that scheme, ignoring relevant information from the model. Our alternative single step approach iteratively updates position and orientation of the CAD model in order to fit its normal vectors with the gradient of the tomographic image. Careful management of the displacement space (SE(3) Lie group) enables us to assess the accuracy of the registration, a must for our applications.

9:10 AM
Atom Probe Tomography Quantization and Autocorrelation Mapping for Studying Grain Boundary Networks and Solute Segregation in Nanocrystalline Alloys: *Ying Chen*[1]; [1]Rensselaer Polytechnic Institute

Solute distribution in nanocrystalline alloys is often measured by Atom Probe Tomography (APT). However, APT does not directly yield grain boundary features. We developed a local spatial autocorrelation-based modeling method to reconstruct nanoscale grain structures and establish solute segregation statistics in nanocrystalline alloys from APT data. Using nanocrystalline Ni-W alloys, we reconstruct the three-dimensional grain boundary network by carrying out two series of APT data quantization, the first probing the anisotropy in the apparent local atomic density and the second quantifying the local spatial autocorrelation. Similar procedures are carried out for local composition. Segregation of solute atoms is revealed, and its correlation with grain boundary locations is examined. This approach enables automatic and efficient quantification and visualization of grain structure and solute segregation in a large volume and at the finest nanoscale grain sizes.

9:30 AM Break

Advances in 3D Materials Modeling: In-situ Experiments and Phase Field Simulations

Wednesday AM | Room: Salon IV
July 13, 2016 | Location: Pheasant Run Resort

Session Chair: Henning Poulsen, Risoe DTU

8:00 AM Invited
In Situ Experiments in X Ray Tomography: *Eric Maire*[1]; [1]Mateis Universite Lyon INSA

This paper aims at presenting a general overview of experimental modalities for in situ experiments in X ray tomography.This will start with some basic observation of systems evolving or transforming with no stress or just a simple initial stimulus. Then evolution due to temperature, stress, electrical stimulation will be shown. Discussion will focus on the different constraints that the peculiarity of X ray tomography acquisition imposes on the sample environment including very high resolution and very fast acqusition. The discussion will also highlight the important scientific breakthrough obtained using these experiments.

8:30 AM
Three-Dimensional Phase-Field Simulation of Concurrent Dendrite Growth and Coarsening During Solidification in Al-Cu Alloys: *Yue Sun*[1]; Ahmet Cecen[2]; K. Aditya Mohan[3]; Xianghui Xiao[4]; Peter Voorhees[1]; [1]Northwestern University; [2]Georgia Institute of Technology; [3]Purdue University; [4]Argonne National Laboratory

The morphological evolution of dendritic microstructures during solidification processes has a strong impact on the properties of the final product. There have been many analytical and numerical models for pure growth and pure coarsening processes, yet few for concurrent growth and coarsening, which is often the case in real-life alloy solidification processes. Using time dependent tomography, the evolution of a dendritic solid-liquid mixture has been measured. We use these structures as initial conditions in a phase-field model of this process, and the results are compared to experiment. The comparison of the morphology is made using interface shape distributions, and a two-point correlation statistical analysis method. The simulation uses a generic phase-field model with CALPHAD free energy functions, which can be easily generalized to other alloys and multiphase systems. The insights in the physics of this growth and coarsening process provide by the comparison between simulation and experiment will be given.

8:50 AM
GPU-Accelerated 3D Phase Field Crystal Simulation of Grain Boundary Motion in Bcc Bicrystal: *Akinori Yamanaka*[1]; Kevin McReynolds[2]; Peter Voorhees[2]; [1]Tokyo University of Agriculture and Technology; [2]Northwestern University

In this study, in order to accelerate three-dimensional (3D) phase field crystal simulation, we develop a phase field code for parallel GPU computing. Using the developed code, we study 3D grain boundary motion in a bcc iron bicrystal. We investigate grain shrinkage behavior in the bicrystal composed of a spherical grain embedded at the center of a single grain. The simulation results show that the spherical grain shrinks by capillary forces and complex dislocation structure are formed at the grain boundary. This study reveals the correlation of the grain boundary motion and the grain boundary dislocation reaction, depending on the initial misorientation between the grains. Furthermore, a comparison of the phase field crystal and molecular dynamics simulations is conducted.

9:10 AM
A Multi-Component Phase-Field Simulation of Ordered Intermetallic Compounds in Low Density Steels: *Alireza Rahnama*[1]; Richard Dashwood[1]; Sridhar Seetharaman[1]; [1]University of Warwick

A 3D phase field model was developed to simulate the evolution of ordered intermetallic compounds in multi-component Fe-C-Mn-Al-Ni low density steels. In this study, the transformation from disordered BCC and FCC structures to an ordered phase through the phase-field method is described. This forms the theoretical foundation for developing a heat-treatment model for microstructure optimisation of the alloys. The variation of order parameters corresponding to each alloying element with aging temperature and holding time was investigated. According to this simulation, Al and Ni contents in the intermetallic compounds tend to increase with the aging time while the Mn content in the intermetallic compounds decreases with that. The effect of both interfacial and elastic strain energies on the precipitate morphology was studied. The simulation results show that the intermetallic precipitates formed in the austenite matrix are much coarser than those formed in the ferrite matrix. This agrees with experimentally reported observations.

9:30 AM Break

Image Processing and Digital Representation of Microstructure: Quantification of Structure and Improvement of Data Quality

Wednesday AM | Room: Salon III
July 13, 2016 | Location: Pheasant Run Resort

Session Chair: David Rowenhorst, Naval Research Lab

10:00 AM Invited
Microstructural Image Analysis using Computer Vision and Machine Learning: *Elizabeth Holm*[1]; Brian DeCost[1]; [1]Carnegie Mellon University

Materials science is, at its core, the science and engineering of microstructure, and microstructural images are the foundational data of materials science. Computational techniques are widely applied both in the acquisition and analysis of microstructural images. When the catalog of possible microstructural features is known, such techniques can take advantage of well-defined feature characteristics to segment, analyze, and compare microstructures with high precision. However, when the features of interest are not known a priori, these methods may become intractable, inaccurate, or fail completely. In contrast, our goal is to develop a general method to find useful characteristics and relationships within and between micrographs without any assumptions about what features may be present. In this project, we develop and apply the ‘bag of visual features’ image representation, based on computer vision concepts, to create microstructural fingerprints that can be used to automatically find relationships in large and diverse microstructural image data sets. For example, the bag of visual features can form the basis for a visual search engine that determines the best matches for a query image in a database of microstructures. Likewise, the microstructural fingerprint can be used to train a support vector machine (SVM) to classify microstructures into one of seven groups with high accuracy. Finally, the microstructural fingerprint can be correlated with quantitative microstructural metrics, thus providing image analysis without the need for segmentation or measurement.

10:30 AM
A New Technique to Estimate the Bias and Precision of Measurements Made from Tomography Scans: *Robert Bradley*[1]; Philip Withers[1]; [1]The University of Manchester

X-ray computed tomography (XCT) is being increasingly used as the basis of non-destructive measurement schemes of quantities such as porosity, defect size and crack growth in materials science applications. However, such measurements are typically presented without an assessment being made of their associated uncertainty, variance or confidence interval. In particular, noise in scan radiographs places a fundamental lower limit on the precision and bias of measurements made on the resulting volumetric data sets. The complete process from scan acquisition to quantification should therefore be viewed as an estimation process. We have adapted the SIMEX statistical technique for bias reduction and variance estimation of such measurements. We demonstrate the efficacy of the technique in simulation studies and on real measurements made using two microtomography systems. Overall SIMEX can provide reliable estimates without taking repeat scans, which can be prohibitive in terms of instrument time or impractical for time-lapse studies.

10:50 AM
Fidelity Analysis of EBSD-Based Orientations and Disorientations Obtained by Two Type of Analyses: (1) Based on the 2D-HT and (2) Based on a Dictionary of Dynamical, Forward-Modeled EBSPs: *Farangis Ram*[1]; Saransh Singh; Stefan Zaefferer[2]; Tom Jäpel[2]; Marc De Graef[1]; [1]Carnegie Mellon University; [2]Max-Planck Institut für Eisenforschung GmbH

The Electron Backscatter Diffraction technique in a scanning electron microscope is a standard technique for capturing backscatter Kikuchi diffraction patterns on a 2D or 3D grid. The patterns are then analyzed to determine the crystal orientation at each grid point. In this work, we present the fidelity analysis of the orientations and disorientations obtained by two methods: (1) the standard 2D Hough transform- (2D HT-) based method and (2) the novel method based on a dictionary of dynamical, forward modeled electron backscatter diffraction patterns. The analyses are performed via descriptive and inferential statistics. For both methods, theoretical patterns with known orientations are processed to resemble experimental patterns. These patterns are the fed into the orientation retrieval algorithm and their retrieved orientations are compared to their true orientations. An analytical accuracy measure based on the Fisher-von Mises distribution is also verified to reliably predict the orientation error.

11:10 AM
MIPAR™: 2D and 3D Characterization Software Designed for Materials Scientists, by Materials Scientists: *John Sosa*[1]; Jacob Jensen[1]; Daniel Huber[1]; Hamish Fraser[1]; [1]The Ohio State University

The materials science community is pursuing an increasing number of experiments which involve the acquisition of three-dimensional multi-modal data. While a variety of instruments have emerged to meet these demands, the software needed to effectively handle multi-modal datasets has not seen as rapid a development. This is understandable since co-registering and fusing pixel-dense electron image data with often sparse, yet multivariate compositional or orientation data can be more challenging than their acquisition. In this work, we present the use of MIPAR™, a unique software suite which has grown to offer a rich set of 2D and 3D materials characterization tools. Among these are tools for user-friendly co-registration, reconstruction, and co-visualization of multi-modal 3D data. They will be presented through their application to characterize nano-scale precipitates captured within STEM tomography and FIB serial-section multi-modal datasets.

11:30 AM
Numerical Descriptors of Polycrystals for Combined High-Energy X-Ray Diffraction Experiments and Polycrystal Computations: *Romain Quey*[1]; Loïc Renversade[1]; [1]Ecole des Mines / CNRS

We describe a methodology for generating polycrystalline microstructures from experimental data obtained by several 3D characterization techniques, that can then be used for crystal plasticity computations using the finite element method (or the FFT method). The microstructures are represented by Laguerre tessellations whose seed positions and weights are set so as to obtain the prescribed experimental grain properties. We provide an efficient implementation of the method and demonstrate how it can be applied to: (i) statistical properties, such as a grain size distribution, (ii) incomplete grain-based properties, for example centroid-volume data obtained by 3DXRD, and (iii) microstructure images obtained by DCT, HEDM or FIB-EBSD. We discuss how well the method performs in these different cases. Finally, we show how the resulting microstructures can be used for polycrystal computations. The presented algorithms are available in the free (open-source) software package Neper (http://neper.sourceforge.net).

11:50 AM
Enhancing Structural Resolution of Lithium-Ion Battery Particles by Multimodal Analysis of TXM and STEM Datasets: *Xiaogang Yang*[1]; Charudatta Phatak[1]; Doga Gursoy[1]; Francesco De Carlo[1]; Vincent De Andrade[1]; Begum Gulsoy[2]; [1]Argonne National Laboratory; [2]Northwestern University

Studying the 3D structure of cathode particle agglomerate in Lithium-ion batteries can help in designing new and improved battery materials. Multiple visualization methods have been used. Scanning electron transmission microscopy (STEM) offers high spatial resolution to depict the morphological details, but can analyze only a thin section of the sample. Transmission x-ray microscopy (TXM) is capable of measuring the whole agglomerate, but at a lower spatial resolution. We are developing algorithms to combine these modalities by using high resolution information from 3D STEM data to enhance the resolution of 3D TXM data. We will present results from the analysis of the same agglomerate first with TXM, then with STEM. By comparing the common region of the registered datasets, we extrapolate the high spatial frequency information in the TXM data using Fourier series methods. Our multimodal analysis approach promises improved spatial resolution for TXM for the analysis of battery particles.

12:10 PM Lunch

Processing-Structure-Property Relationships in 3D: Experimental Investigation and Modeling of Deformation and Failure

Wednesday AM
July 13, 2016

Room: Salon IV
Location: Pheasant Run Resort

Session Chair: Eric Maire, Mateis Universite Lyon INSA

10:00 AM Invited
Dark-Field X-Ray Microscopy: Multiscale Structure and Stress Mapping: *Henning Poulsen*[1]; Frederik Stöhr[1]; Sonja Ahl[1]; Annika Diederichs[1]; José Trujillo[1]; Hugh Simons[1]; Anders Jakobsen[1]; Søren Schmidt[1]; Wolfgang Pantleon[1]; Jakob Bowen[1]; Wolfgang Ludwig[2]; Carsten Detlefs[2]; [1]DTU; [2]ESRF

The status of dark field x-ray microscopy is provided. Using a synchrotron beam and an x-ray lens in the diffracted beam magnified 2D images of embedded grains, domains and dislocations which fulfill the diffraction condition can be generated. 3D structural mapping is provided by rotating the sample and making tomography-type reconstructions, while stress mapping is achieved by scanning the objective. Approaches for multiscale mapping, where one "zooms in and out" on objects in 3D, are presented [1]. Specifications for a recently commissioned microscope at beamline ID06 at the European Synchrotron Radiation Source will be given. Finally the use of dark field x-ray microscopy will be illustrated by example. References:[1] Simons et al. Nature Comm. 6, 6098 (2015)

10:30 AM

Dynamic In Situ Loading of Materials during Synchrotron 3D Tomographic Imaging: *Brian Patterson*[1]; Nikhilesh Chawla[2]; Sudhanshu Singh[2]; Angel Overjero[2]; Jason Williams[2]; Xianghui Xiao[3]; Kevin Henderson[1]; Robin Pacheco[1]; Nikolaus Cordes[1]; James Mertens[1]; [1]Los Alamos National Laboratory; [2]Arizona State University; [3]Argonne National Laboratory

Understanding the effects of material composition, geometry, aging, and processing upon the overall material performance requires a detailed understanding of their initial morphology and how the morphology changes under external stimuli. Synchrotron light sources, such as the APS, afford materials researchers unprecedented X-ray flux to help unravel these complex materials science challenges. Coupling this high flux with a high speed camera means that a full 3D tomographic data can be collected in ~0.25 second with a ~five micrometer voxel size. A sample loading cell makes it possible to study the dynamic in situ deformation of materials at a 10-2 strain rate. The imaging of polymer foams during compression was completed and modeled using Abaqus. Tomographic imaging of 3D printed materials during tension shows the 3D flow of the glass filled nylon material and the delamination of the filler material and the polymer binder during the plastic flow and breakage.

10:50 AM

In Situ X-Ray Tomographic Characterisation and Modeling of Low Cycle Fatigue Crack Behavior in a Cast Al Alloy at High Temperature: *Sébastien Dézécot*[1]; Jean-Yves Buffiere[1]; vincent Maurel[2]; Fabien Szmytka[3]; Alain Koster[2]; [1]INSA de Lyon; [2]MINES ParisTech; [3]PSA Peugeot Citroen

The aim of this work is to study the initiation and propagation of cracks in a Lost Foam cast $AlSi_7Cu_3Mg$ aluminum alloy using synchrotron X ray tomography during in situ isothermal (250°C) Low Cycle Fatigue (LCF) tests. A pore free material (produced by hot isostatic pressure) is also investigated for comparison. 3D microstructurally realisitic meshes of the material are generated from the tomographic images to perform 3D elasto-viscoplastic simulation of the material during LCF tests. Crack initiation occurs in the bulk of the samples on secondary particles located at the pore vicinity. The local inelastic strain in these regions appears as a good indicator for predicting crack initiation localization. Crack initiation, secondary particules failure or decohesion and subsequent crack paths are seen to be correlated with modeled high stress triaxiality and inelastic strain areas. Local failure criterion is finally discussed on the basis of 3D analysis of crack growth.

11:10 AM

Microstructurally-Short Crack Growth Driving Force Identification: Combining DCT, PCT, Crystal Plasticity Simulation and Machine Learning Technique: *Andrea Rovinelli*[1]; Michael Sangid[1]; Ricardo Lebensohn[2]; Wolfgang Ludwig[3]; Yoann Guilhem[4]; Henry Proudhon[5]; [1]Purdue University; [2]Los Alamos National Lab; [3]ESRF; [4]ENS de Cachan; [5]MINES ParisTech

Identifying the Microstructurally-Short Crack (MSC) growth driving force of polycrystalline engineering alloys is a critical need in assessing performances of materials subject to fatigue load and to improve both material design and component life prediction. However, due to (i) the lack of “cycle-by-cycle” experimental data, (ii) the complexity of MSC growth phenomenon, and (iii) the incomplete physics of constitutive relationships, only simple driving force metrics, inadequate to predict MSC growth, have been postulated. Based on experimental results by Ludwig, Guilhem, et al., “cycle-by-cycle” data of a MSC propagating through a beta-metastable titanium alloy are available via phase and diffraction contrast tomography. To identify the crack driving force, we developed a framework utilizing the aforementioned experimental results and FFT-based crystal plasticity simulations (to compute micromechanical fields not available from the experiment). These results are combined and converted into probability distributions for use in a Bayesian Network.

11:30 AM

Modelling of the Plastic Anisotropy of Steel under Different Strain Rates and Temperatures by Crystal Plasticity Finite Element Method: *Junhe Lian*[1]; Sihwa Sung[1]; Deok-Chan Ahn[2]; Dong-Chul Chae[2]; Sebastian Münstermann[3]; Wolfgang Bleck[1]; [1]RWTH Aachen University; [2]POSCO; [3]Jülich Research Centre

The aim of this study is to propose a methodology to predict the plastic anisotropy of bcc steels by using the crystal plasticity finite element method. Experimental characterization of the plastic anisotropy on tensile tests of a ferrite stainless steels was conducted at different temperatures and strain rates. For the anisotropy prediction, 3D representative volume elements (RVE) are employed. Extensive study is performed on the construction of the RVE including the effects of texture discretization, mesh discretization in single grain and grain morphology. A new strategy to calibrate the crystal plasticity parameter is proposed, with which the flow curves of the material at different strain rates are naturally captured. The method is also extended to different temperatures for the prediction of the thermal effect on the plastic anisotropy of steels.

11:50 AM

4D Monitoring of Fibre Failure on CFRP by In Situ Ultrafast X-Ray Computed Tomography: *Serafina Consuelo Garcea*[1]; Philip Withers[1]; [1]The University of Manchester

In situ ultrafast synchrotron X-ray computed tomography has been used to investigate the evolution of fibre failure in a toughened particle carbon/epoxy under quasi-static load. Computed tomography is widely recognized as a powerful technique to inspect damage in composites. However, single static scans exhibit some limitations related to the inability to capture instable mechanisms preceding failure and to modify failure micromechanisms when coupons are hold under a constant load during static scans. Ultrafast computed tomography was successfully used in this work to overcome the limitations mentioned above. Double end notch coupons with a cross-ply layup were progressively loaded (in tension) and continuously scanned. Fibre breaks accumulation was mapped at different percentages of the ultimate tensile strength, and more interestingly in the last 11 seconds before failure. Results provide important insights into the fundamental failure mechanisms as well as a guidance to inform models and improve material performance.

12:10 PM Lunch

Future Directions and Challenges in 3D Materials Science: Experimental Capabilities

Wednesday PM	Room: Salon III
July 13, 2016	Location: Pheasant Run Resort

Session Chair: Dorte Jensen, DTU Risø

2:00 PM Invited

MultiBeam Tomography: Current and Future Capabilities: *Tresa Pollock*[1]; William Lenthe[1]; McLean Echlin[1]; [1]University of California Santa Barbara

The current capabilities of femtosecond lasers, in combination with focused ion beams, for generation of mm-scale 3D datasets will be reviewed. Across a spectrum of materials classes, surface damage and the capabilities of the TriBeam approach for 3D data acquisition has been characterized. Current challenges in acquisition, reconstruction and analysis of multimodal datasets, generated within a single platform and across platforms, will be discussed. Future possibilities for combining beams and increasing the efficiency of 3D dataset generation will be considered.

2:30 PM

Multi-Scale 3D Experimental Workflow of an Aluminum 7075 Alloy: *Arno Merkle*[1]; Nikhilesh Chawla[2]; Sudhanshu Singh[2]; Lorenz Lechner[1]; [1]Carl Zeiss X-ray Microscopy; [2]Arizona State University

Here we detail a multi-scale tomographic study on an aluminum 7075 alloy, containing precipitates and inclusions, which has benefitted from characterization of the same sample volume across multiple length scales and the subsequent quantification and analysis (shape, size, etc.). An efficient 3D correlative tomography workflow is presented, that utilizes 3D X-ray microscopy (XRM), a non-destructive sub-micrometer tomographic imaging approach, to guide focused ion beam and scanning electron microscopy (FIB-SEM) to reveal specific targeted sub-surface regions of interest at high resolution also in 3D. This coordinated approach, enabled by the emergence of an integrated, modern workflow environment points to the future of correlation in 3D across modalities and length scales. Here we discuss the scientific challenges and need for such multi-scale studies as well as the experimental strategies required in making such studies a common reality.

2:50 PM
Advanced In Situ Loading Environments for Synchrotron X-Ray Diffraction Experiments: *Paul Shade*[1]; Todd Turner[1]; Jay Schuren[1]; Basil Blank[2]; Joel Bernier[3]; Shiu Fai Li[3]; Jonathan Lind[3]; David Menasche[4]; Robert Suter[4]; Ulrich Lienert[5]; Peter Kenesei[6]; Jun-Sang Park[6]; Jonathan Almer[6]; Darren Dale[7]; Ernest Fontes[7]; Matthew Miller[8]; [1]Air Force Research Laboratory; [2]PulseRay; [3]Lawrence Livermore National Laboratory; [4]Carnegie Mellon University; [5]DESY; [6]Advanced Photon Source; [7]Cornell High Energy Syncrotron Source; [8]Cornell University

High energy x-ray characterization methods hold great potential for gaining insight into the behavior of materials and providing comparison datasets for the validation and development of mesoscale modeling tools. A suite of techniques have been developed by the x-ray community for characterizing the 3D structure and micromechanical state of polycrystalline materials; however, combining these techniques with in situ mechanical testing under well characterized and controlled boundary conditions has been challenging due to experimental design requirements. In this presentation, we describe advanced in situ loading environments that have been developed for communal use at the Advanced Photon Source and the Cornell High Energy Synchrotron Source. Example 3D datasets that have been collected using this hardware and their application for materials modeling efforts will be discussed.

3:10 PM Break

Future Directions and Challenges in 3D Materials Science: Synergy of Experiments and Modeling and Industry Application

Wednesday PM — Room: Salon IV
July 13, 2016 — Location: Pheasant Run Resort

Session Chair: Michael Groeber, AFRL

2:00 PM Invited
3D Analysis in the Research and Development of Steel Products - Current Topics and Future Anticipations: *Akira Taniyama*[1]; [1]Nippon Steel

With the development of the new powerful 3D characterization and analysis techniques it has become feasible to advance from coarse scale, average investigations to detailed investigations of also internal structures on the micron or even submicron scale. It is now possible to characterize and analyze the structural arrangement, the shapes of defects such as voids and cracks, and the crystallographic grain structure in raw steel materials and steel products. Therefore, it is expected to apply these new methods and results to optimize of steel making processes and to improve the mechanical properties of steel products. In this talk, the role of 3D characterization and analysis in the R&D of steel products and of the steel making process will be presented. Furthermore, future anticipations for 3D analysis which are suitable for steel material research will be discussed.

2:30 PM
Comparison of Experiment and Simulation in Deformation of Polycrystals: *Anthony Rollett*[1]; Jon Lind[2]; Reeju Pokharel[3]; Ricardo Lebensohn[3]; Robert Suter[1]; [1]Carnegie Mellon University; [2]Lawrence Livermore National Laboratory; [3]Los Alamos National Laboratory

We summarize the current state of comparisons between experiments and simulations of deformation of polycrystalline materials. It is important to demonstrate that we can validate crystal plasticity simulations in order to relate damage initiation such as cracks and voids to extreme values in stress, for example, as they relate to microstructural features such as triple lines. Specific examples will be given for tensile tests on pure copper and pure Zr, using High Energy Diffraction Microscopy (HEDM). The micro-mechanical response was simulated with a spectral method based on Fast Fourier transforms (FFT). In general, both experiments and simulations show that hot spots in stress or elastic energy density occur close to grain boundaries, triple lines and quadruple points. Although correlations are found between hot spots and interfaces, special boundaries do not appear to play any role and, instead, differences in plastic response across boundaries appear to dominate.

2:50 PM
3D Materials Science and Engineering: Progress Toward Engineering Capabilities: *Dennis Dimiduk*[1]; Sean Donegan[1]; Michael Jackson[1]; Michael Uchic[2]; Michael Groeber[2]; [1]BlueQuartz Software, LLC; [2]Air Force Research Laboratory

About 15 years ago, research and development into 3d-MSE tools increased as instruments and computing capabilities improved. However, industrial design, manufacturing and materials engineering is slow to adopt the tools. Here we suggest five domains for 3d-MSE development: i) experimental techniques/instruments and sample attributes; ii) 3d digital data acquisition; ii) data processing and segmentation; iv) analysis and quantification of data; and, v) representation of 3d structures and model building. These five areas are critically assessed via selected examples from robotic serial sectioning, focused ion beam serial sectioning, and high-energy X-ray diffraction sectioning methods, to identify aspects for more focused development. From the assessment we suggest that 3d-MSE is a systems engineering challenge requiring iterative holistic development, yet the 3d-MSE community proceeds largely along segregated lines of interest. We conclude that the cost of 3d-MSE information and the slow-to-develop knowledge base of skilled practitioners are also major obstacles to widespread adoption.

3:10 PM Break

Panel Discussion

Wednesday PM — Room: Salons III&IV
July 13, 2016 — Location: Pheasant Run Resort

Session Chair: George Spanos, TMS

3:30 PM Panel Discussion
Panelists:
Alexis Lewis, NSF
Tresa Pollock, University of California, Santa Barbara
Akira Taniyama, Nippon Steel
Paul Dawson, Cornell University
Jon Almer, Argonne National Laboratory
Eric Maire, Mateis Universite Lyon INSA
Dennis Dimiduk, Blue Quartz Software, LLC

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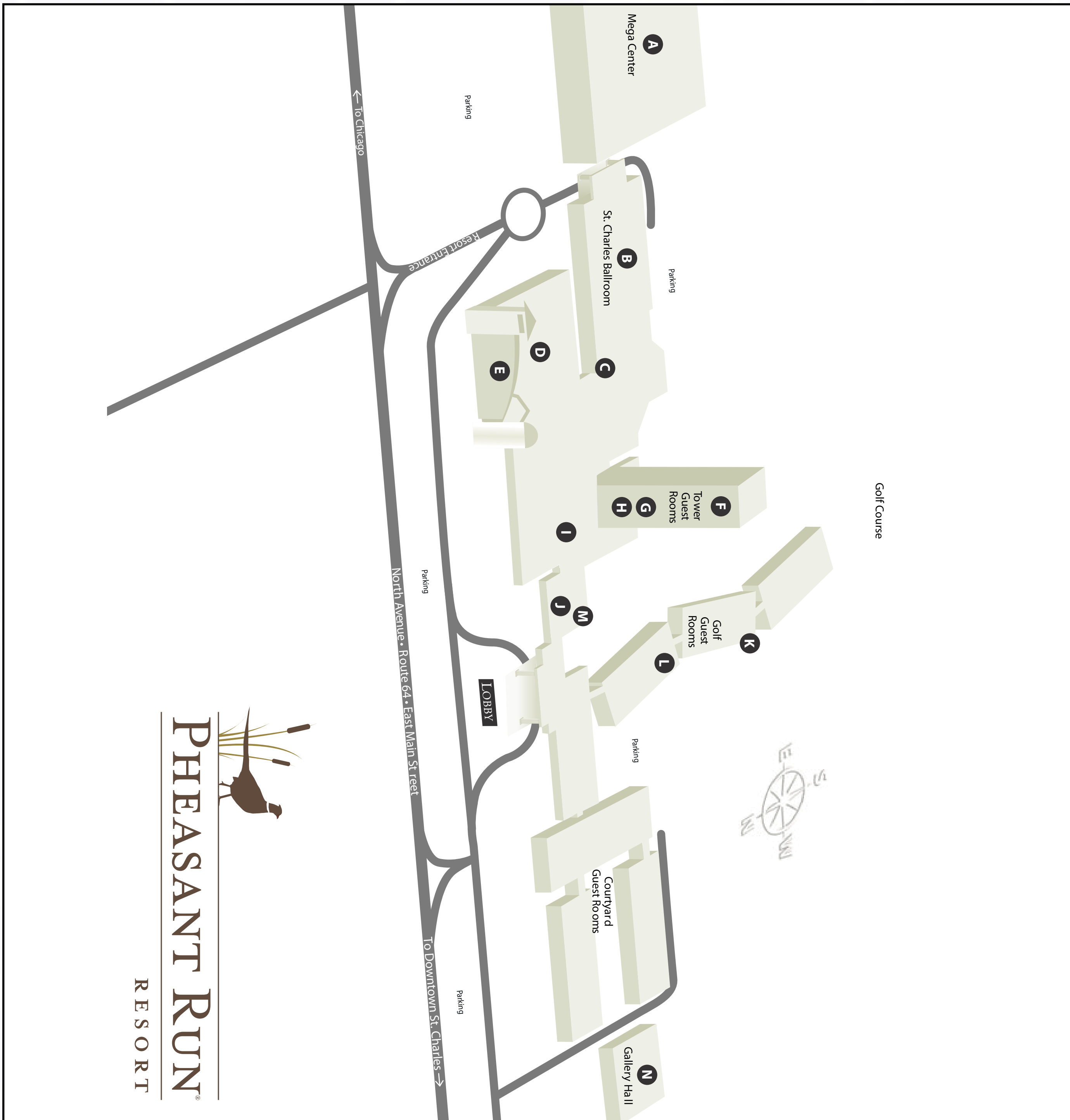

Pheasant Run Resort Map

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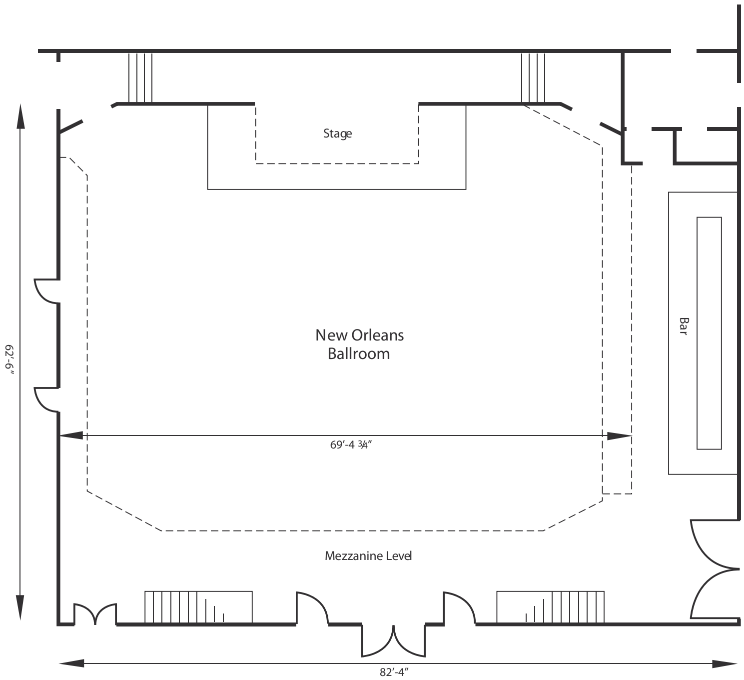
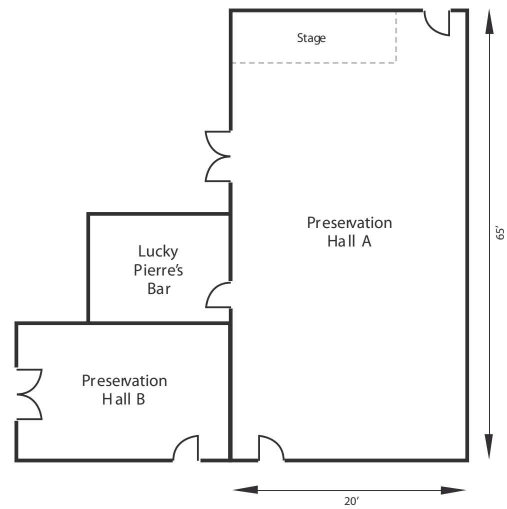
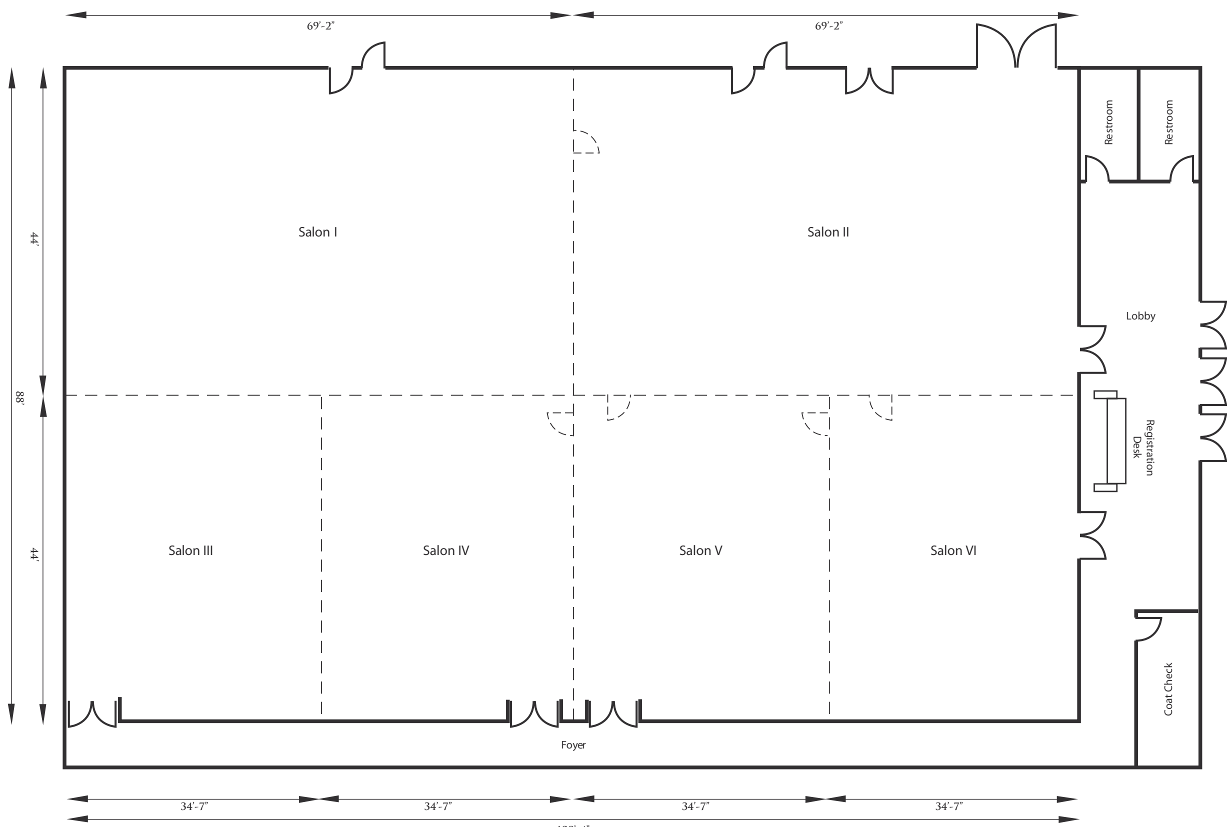
New Orleans Ballroom & Preservation Hall





St. Charles Ballroom



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- September 1, 2016: Manuscripts Due for Proceedings
- October 2016: Registration Opens

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