The 3rd International Congress on 3D Materials Science 2016

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

FINAL PROGRAM

Sponsored by:

www.tms.org/3DMS2016
Unlocking crystallographic information in your lab

ZEISS LabDCT

LabDCT

Bringing synchrotron technology to the laboratory

Directly visualize 3D crystallographic grain orientation in a non-destructive tomography environment with LabDCT for ZEISS Xradia 520 Versa 3D X-ray microscopes. Combine grain orientation information with microstructural features and open new possibilities for characterization of damage, deformation and growth mechanisms for 3D materials science.

pages.zeiss.com/LabDCT


Scan code to view direct visualization of a beta-Ti alloy with crystallographic information showing over reflections for 500 grains simultaneously.
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.
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<td>Welcome Reception</td>
<td>6:30 p.m. to 7:30 p.m.</td>
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<td>Break</td>
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<tr>
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<td>8:00 a.m. to 5:00 p.m.</td>
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<td>Break</td>
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<td>Exhibition Dismantle</td>
<td>After 3:30 p.m.</td>
<td>St. Charles Ballroom Salon II</td>
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<td>Panel Discussion</td>
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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**

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<td>Sunday</td>
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</tr>
<tr>
<td>Wednesday</td>
<td>7:30 a.m. to 4:30 p.m.</td>
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</tbody>
</table>

**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.

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</tr>
<tr>
<td>Wednesday</td>
<td>8:00 a.m. to 3:30 p.m.</td>
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**CALL FOR ABSTRACTS**

**Deadline:** September 30, 2016

4th World Congress on Integrated Computational Materials Engineering (ICME 2017)
May 21–25, 2017 • Marriott Ann Arbor Ypsilanti at Eagle Crest
Ypsilanti, Michigan, USA

**DON’T MISS THIS OPPORTUNITY TO SHARE YOUR WORK AND CONNECT WITH LEADERS IN ICME.**

www.tms.org/ICME2017/CFA
ABOUT THE CONGRESS

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.

Avizo®

3D analysis software

Avizo is a powerful, multifaceted 3D software for exploring and understanding materials structures and properties.

- Flexible data import
- State-of-the-art visualization
- Advanced image processing
- Powerful image segmentation tools
- Measurement and quantitative analysis
- High quality presentation and animation

Visit us at 3DMS 2016 to learn more about our 3D software solution.

Avizo3D.com
TMS would like to thank the following Corporate Sponsors and Exhibitors for their gracious support of the event:

**GOLD SPONSOR**

Carl Zeiss Microscopy, LLC

Throughout the world, ZEISS stands for the highest quality and reliability. Carl Zeiss Microscopy is part of the Carl Zeiss group, a leading organization of companies operating worldwide in the optical and opto-electronic industry. As the world’s only manufacturer of light, X-ray and electron/ion microscopes, Carl Zeiss Microscopy offers tailor-made systems for industry, materials research and academia. A dedicated and well-trained sales force, an extensive support infrastructure and a responsive service team enable customers to use their ZEISS microscope systems to their full potential.

**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
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.

Anti-Harassment

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

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

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

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

Photography and Recording

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

Any recording of sessions (audio, video, still photography, etc.) intended for personal use, distribution, publication, or copyright without the express written consent of TMS and the individual authors is strictly prohibited. Attendees violating this policy may be asked to leave the session.

Antitrust Compliance

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

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 3D Materials Science 2016

TECHNICAL PROGRAM

www.tms.org/3DMS2016
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$_f$ 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; Jianguo Hao; 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 Kobayashi1; Aya Kouno1; Tomohiko Matsuyma1; Hirokky Toda2; Hiromi Miura3; Osamu Kuwazuru4; Toyohashi University of Technology; Kyushu University; 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 Ozturk1; Ross Cunningham2; David Menasche3; Robert Suter4; Anthony Rollett5; 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.
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 directly compared with CDI images to reveal the role of the interface in the phonon scattering. Here, we discuss how multi-million atom molecular dynamics simulations, in core-shell structures where interfacial effects can play an important role in phonon scattering. We present the case of using dark field x-ray microscopy to map dislocations within a 400 µm thick diamond sample. Potential applications are outlined.

11:20 AM Image-Based Finite Element Analysis for Fatigue of Cast Aluminum Alloy: Osamu Kawazuru; Masakazu Kobayashi; Hiroyuki Toda; University of Fukui; Toyohashi University of Technology; 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; Samantha Daly; 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; Mathew Cherukara; Ross Harder; Jesse Clark; Nicola Ferrier; Thomas Peterka; Subramanian Sankaranarayanan; Argonne National Laboratory; 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 bimetallic (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
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; Yoshiki Seno; Daigo Setoyama; 

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 \( \times \) 95f.m. 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\(^2\) voxels at the voxel size of 1-2\(\times\)956f.m under stress is obtained by 33 Hz diffraction image data collection synchronized with the 20/176/s endless sample rotation.

12:20 PM Lunch

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**TECHNICAL PROGRAM**

**10:20 AM Break**

**10:40 AM**

Mapping Nano-Scale Strain and Orientation in Multiferroic Materials with Dark-Field X-Ray Microscopy: Hugh Simons; Sonja Ahl; Anders Jakobsen; John Daniels; Dragan Damjanovic; Carsten Detlefs; Henning Poulsen; 

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 Guerinchaud; Henry Proudhon; Wolfgang Ludwig; Samuel Forest; 

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 compared 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; Robert Carson; Paul Dawson; Matthew Miller; 

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; Thilo Morgeneyer; Frembert Nizey; Lucien Laiaraindrasana; Peter Cloetens; 

Computed X-ray tomography has become routine to study many kinds 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
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 Pagan1; 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 Lebensohn1; Pokharel Reej1; Bjorn Clausen1; Cristina Garcia-Cardona1; Evan Lieberman1; Chris Chen1; Marian Anghel2; Timothy Ickes2; James Hunter3; Robert Suter2; Anthony Rollett1; Thibault Taillandier-Thomas3; Martin Poncelet1; François Hild1; Stéphane Roux1; Marc De Graef1; Charles Bouman2; K. Aditya Mohan1; Carnegie Mellon University; Cornell University; Thales; University of Saclay; Lawrence Livermore National Laboratory.

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.

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 Bouman1; 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 implement 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 reconstruct 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 Prabhat1; Marc De Graef1; Charles Bouman2; K. Aditya Mohan1; Carnegie Mellon University; 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, $A(r)$. 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 divergenceless condition to reconstruct all three components of $A(r)$. 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; Jitesh Vasavada; Hirishkesh Bale; Christian Holzner; Leah Lavery; Sushil Mishra; Asim Tewari; 1IIT Bombay; 2Carl 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 Sauer; David Menasche; 1Carnegie Mellon University

We describe the motivation for and the implementation of calculations of diffracted beam intensities appropriate for near-field High Energy Diffraction Microscopy (n-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 also be applied to predict n-HEDM diffracted beam intensities appropriate for near-field High Energy Diffraction Microscopy (n-HEDM) and thereby may lead to more precise estimates of elastic lattice strains.

4:40 PM Invited
High-Resolution X-Ray Computed Tomography at SPring-8 and Improvements of Imaging Properties: Akhisra Takeuchi; Kentaro Uesugi; Hiroyuki Toda; Masakazu Kobayashi; 1JASRI / SPring-8; 2Japan Synchrotron Radiation Research Institute (JASRI)/SPring-8; 3Kyushu University; 4Tokyo 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 synchrotron-Radiation Tomography Investigation: Yazid Madi; Juan Garcia; Thilo Morgencery; Henry Proudhon; Jacques Besson; 1EPF-Ecole d’in génieurs / Centre des Matériaux Mines ParisTech; 2Centre 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; Armand Beaudoin; 1University 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 by prism slip.

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

P-1: 2-Dimensional Synchrotron Radiation Diffraction Measurement for 3-Dimensional Distribution of Strains with Sub-mm Spatial Resolution:
Hidehiko Kimura; Daigo Setoyama; Satoshi Yamaguchi; 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; Veera Sundararaghavan; 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; Nirmal Singh; 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; Takashi Asada; Satoshi Yamaguchi; Takeshi Uyama; Yujiro Hayashi; 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; Anthony Rollett; 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; Dani Liu; Bahareh Shikababjahromi; Chelsea Knittel; David Breen; Genevieve Dion; Antonios Kontsos; Department of Mechanical Engineering and Mechanics, Drexel University; College of Computing and Informatics; Shima Seiki Haute Technology Laboratory, ExCITE Center, Drexel University

Smart textiles constitute an emerging class of architectural 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 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: Yinbin Zhang; A. Lyckegaard; P. Reischig; C. Holzner; E. Lauridsen; Technical University of Denmark; Xnovo Technology ApS; 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 present 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-9: 3D Virtual Heterogeneous Microstructure for Real Particulate Materials Modeling: Yang Lu1; Stephen Thomas3; 1Boise 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, Ann model, with irregular shape particles is proposed. The Ann 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 material matrix 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 Puente1; Dinc Erdeniz2; Julie Fife2; Xianghui Xiao3; David Dunand3; 1Northwestern University; 2Paul Scherrer Institut; 3Argonne 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 Al-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 Bale1; Marty Leibowitz2; Sergey Etchin3; Luke Hunter1; Benjamin Hornberger1; Leah Lavery1; Robert Ritchie2; Brian Cox2; David Marshall2; 1Carl Zeiss X-ray Microscopy, Inc.; 2University of California, Berkeley; 3Teledyne 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 Daudin1; Sofiane Terzi2; Pierre Lhuissier1; Marco Di Michiel1; Mario Scheel1; Elodie Boller1; Luc Salvo1; 1Université Grenoble Alpes, SIMAP; 2European Space Agency; 3ESRF-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 final 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 Rahnamai1; Alireza Rahnamai1; Isfahan University of Technology; 2University 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 mismatch 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 Loughnane1; Michael Uchic2; Michael Groeber2; 1Mound Laser & Photonics Center, Inc.; 2Air 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 proposed, 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 Stark1; Simon Mays2; Jo Soafar3; Sonia Zakrzewska1; 1University of Southampton; 2English 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; Arthur Sonzogni; Olivier Guiraud; Pierre
Latil; 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; Jun-Sang Park; Peter Collins; Adam
Pilchak; Aaron Stebner; Colorado School of Mines; Argonne National Laboratory; Iowa State University; 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; Gregory Rohrer; Anthony Rollett; Carnegie
Mellon University
The Potts Model of grain growth was adapted for the purpose of simulating
abnormal grain growth (AGG) resulting from grain boundary complexation
transitions. The transition in grain boundary structure between specific
complexation 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: Al-Materials Science to Predict Stress-Strain Curve: Yoshitaka
Adachi; Sunao Sadamatsu; 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; 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; Andrew
Petersen; Harshad Paranjape; Ashley Bucek; Aaron Stebner; Colorado School of Mines
High Energy X-ray Diffraction Microscopy (HEDM) provides 3D
countination 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 digital 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; Singh Dileep; Peter Kenesei;
Jonathan Almer; John Hryn; 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; Gregory Rohrer; Anthony Rollett; 1National Institute of Standards and Technology; 2Carnegie 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; Maider Iturrondobeitia2; Julen Ibarretxe; Pello Jim bert1; 1University 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, 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 Papillon2; Eric Maire2; Olivier Ondel2; Damien Fabrègue; Michel Perez; 1INSa de Lyon; 2Université 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 determine 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 Sasaki1; Akinori Yamanaka1; Shin-ichi Itô1; Hiromichi Nagao2; 1Tokyo University of Agriculture and Technology; 2Earthquake 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 Chen1; Mingjie Li1; 1Rensselaer 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 Zhang1; Stefan Poulsen2; Peter Voorhees2; Henning Poulsen2; 1Technical University of Denmark; 2Northwestern 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: Jia-Yi Huo1; Shota Horikawa1; Koji Kakehi1; 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 Zhang1; Chi Xu2; Jun-Sang Park1; Hemant Sharma1; Jonathan Almer1; Meimei Li1; 1Argonne National Lab; 2University 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 Herzing1; 2NIST
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 Hirayama1; Hiroyuki Toda1; Kentaro Uesugi1; Akihisa Takeuchi1; 2Kyushu University; 3Japan 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 Paranjape1; Ashley Buscek1; Darren Dale1; Joel Bernier1; Aaron Steiner1; 2Colorado School of Mines; 3Cornell University; 4Lawrence 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 Fayard1; Pierre Latil1; Arthur Sonzogni1; Olivier Guiraud1; Moreno Trlin1; 2NOVITOM
X-ray micro-tomography can provide the microstructural 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 Hiremath1; Swamendu Bhattacharya1; Jigar Goda1; Anirban Guha1; Asim Tewari1; 2IIT 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. Xiating Zhang1; Gregory Rohrer1; 2CMU
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 Guillen1; Zilong Hua1; Heng Ban1; 2Idaho National Laboratory; 3Utah 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 x 25µm x 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: Investigation of Orientation Relationship and Growth Direction of Beta-Mn Phase in Austenite-Based Lightweight Steels Using 3D Microstructure Reconstruction: Keunho Lee; Siwook Park; Sang Sub Han; Seong-Jun Park; Kyu Hwan Oh; Heung Nam Han; 1 Seoul National University; 1 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; Noel Nuhrer; Gregory Rorher; 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; 1ENSMP

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 (ensemble cases).

P-45: Methods for Determining Integral Mean Curvature of Grain Boundaries in 3D Reconstructed and Simulated Structures: Robert DeHoff; 1 David Rowenhorst; 1 Burton Patterson; 1 Catherine Sahi; 1 University of Florida; 1 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 Yoshioka1; Masahiro Ishida1; Tomokazu Yamamoto1; Kazuhiro Yasuda1; Syo Matsumura1; Shigeru Kimura1; 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: Sutipong Mandal1; Anthony Rollett1; 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 flowsoftening 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 Chizhko1; 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 units. 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 Shi1; 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 Tucker1; Tyler Weihing2; Michael Groeber2; Adam Pilchak1; Exponent1; 3Southwestern Ohio Council for Higher Education; 4Air 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 EBSP 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-Based Superalloys: Ryan Harrison1; Patrick Callahan1; Tresa Pollock2; Marc De Graef1; Carnegie Mellon University; 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. Previous 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 Jasiak1; Sabrina Nilufar1; Gabriela Couvertier Santos1; 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 Brinell 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 transmission 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.
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Crystal symmetry are presented. We compare and contrast the spiral slit system and the conical slit system Diffraction technique using monochromatic x-ray has been widely used to unique features of neutrons as a probe for condensed matter research. Of these promising techniques and sophisticated instrumentation based on the vector field reconstructions. However, only the current advent of the first resolved quantification of structures beyond direct image resolution or magnetic domains, spatially 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.

Modern pulsed spallation neutron sources enable a new generation of neutron imaging instruments profiling 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.

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, powder,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.

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.

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.

The OO 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.

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.

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P-57: One Approach for an Out-of-ROI Reconstruction: Valeriy Titarenko; 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; Stephen Langer; NIST

The OO 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: Hiyoshi Toda; Han Li; Dowon Seo; Rafael Batters; Osamu Kuwazuru; Kyushu University; Tecnologico de Monterrey; Fuku 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: Sebastien Pinson; Remy Dendievel; Cécile Davoine; Audrey Guyon; Grenoble INP; ONERA-The French Aerospace; Sinteetext 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 Rao1; Ross Cunningham1; Tugce Ozturk1; Jaaako Suni2; Cagatay Yanar3; John Siemons3; Deborah Wielamy3; Anthony Rollett1; Carnegie Mellon University; 1Alcoa

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 Barbear1; Kenneth Sabo1; Michael Tims1; Daniel Widdis1; 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 Donegan1; Mike Jackson1; 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 Burca1; W. Kockelmann1; J. Kelleher1; S. Kabra2; S.Y. Zhang3; J.A. James1; T. Minniti1; F. Montesinos-Pousolz2; J.B. Nightingale1; E. Yang1; STFC Rutherford Appleton Laboratory, ISIS Facility; 1The Open University, Milton Keynes, UK; 2STFC 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 format material 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 Zhang1; Nicholas Kotov1; Qing Zhu2; 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 Madison1; T. Rodgers1; V. Tikare1; 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 Vasavada1; Saurabh Arvariya2; Sushil Mishra1; Asim Tewari1; 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 discretor 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 Tatarenko1; 1University 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 suppresses 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 Jespersen1; Monica Emerson1; Anders Dahl1; Knut Conradsen1; Lars Mikkelsen1; 1Technical 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 wound 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 fibre misalignment was linked to experimental measured compression strength values.

P-70: Simulation of Controlling System of Shape Memory Nanotweezers: Peter Lega1; Victor Koleodov1; 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 nanindustry, 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 Jensen1; John Sosa1; Daniel Huber1; Gopal Viswanathan1; Robert Williams1; Hamish Fraser1; 1The 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 interconnection 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 AlMn0.5NbTa0.5TiZr, electron tomography using STEM-HAADF micrographs and super-X XEDS spectral images was utilized.

P-72: Stereological Constraints on Three-Point Correlation Functions: Jitesh Vasavada1; Sushil Mishra1; Asim Tewari1; 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 Lekahl1; 1 MIST

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 Narula1; Sushil Mishra1; Asim Tewari1; IIT Bombay

Crystalllographic 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 crystalllographic 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).
We studied transformational faulting from olivine to spinel in Mg$_2$GeO$_4$, an

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 characterisation), 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; Tony Yu; Mark Rivers; Alexandra Schubnel; Nadege Hilairet; Fabrice Satya Ganti: 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 4Zt 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 4Zt 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: Yiwei Meng; Jian-Min Zuo; University of Illinois at Urbana-Champaign

We report on a high resolution and low-dose scanning electron nanodiffraction (SND) 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. Previously we reported on a prototype instrument. Now, we've achieved a new tool is presented, which enables the three-dimensional reconstruction, visualization and quantification of dislocation densities and dislocation structures 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 CT tool is presented, which enables the three-dimensional reconstruction, visualization and quantification of dislocation densities and dislocation structures. The instrument's capabilities will be demonstrated through thin film analyses.

P-79: Volumetric Elemental Imaging and Quantification by Confocal X-Ray Fluorescence: James Mertrens; Brian Patterson; Nikolaus Cordes; Kevin Henderson; Jeffrey Griego; Thomas Day; Derek Schmidt; George Havrilla; 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 JACOMÉ; Kai Pothkow; Olaf Paetsch; Hans-Christian Hege; Federal Institute for Materials Research and Testing (BAM); 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 filament 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 CT 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 Mertrens; Amy Clarke; Brian Patterson; Ricardo Lebensohn; Kevin Henderson; Damien Tourret; Clarissa Yablinsky; John Gibbs; Seth Imhoff; 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 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.

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.
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 of 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

July 12, 2016

Room: Salon III

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 Lienert1; Wolfgang Pantleon2; 1Deutsches Elektronen-Synchrotron; 2Technical 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 Buffiere1; 1Universite 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 Pokharel1; Donald Brown2; Ricardo Lebensohn3; 1Los Alamos National Laboratory 23D 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 processing stages, during, and after development 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 Burnett1; Tom Slater2; R Bradley2; S Haigh2; P Withers3; 1Manchester University/FEI; 2University 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 Menasche1; Paul Shade2; TJ Turner2; Ulrich Lienert3; Joel Bernier4; Darren Pagan5; Peter Kenesel1; Jun-Sang Park1; Robert Suter1; 1Carnegie Mellon University; 2Air Force Research Lab; 3Deutsches Elektronen-Synchrotron; 4Lawrence Livermore National Laboratory; 5Argonne 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; Christian Holzner; Florian Bachmann; Kenneth Nielsen; Leah Lavery; William Harris; Peter Reischig; Allan Lyckegaard; ¹Xenovio Technology ApS; ²Carl 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 correlative coherently to 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 Worsell; Dayakar Penamadu; Anton Tremis; Nikolay Kardjilov; Ingo Manke; Markus Strobil; ¹European Spallation Source; ²University of California at Berkeley; ³Helmholtz 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 Micromotography and Digital Volume Correlation: Thanh Tung Nguyen; José Bolívar; Julien Rethore; Marion Fregonese; Jerome Adrien; Jean-Yves Buffiere; ¹LaMCoS INSA Lyon, CNRS; ²MATEIS-INSa Lyon, CNRS; ³LaMCoS 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 aluminium matrix and Cu particles and that stress corrosion cracks colonies are obtained. The micromotography 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
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 Pereoloma1; Kun Yan2; Klaus-Dieter Liss3; 1University of Wollongong; 2University of Manchester; 3Australian Nuclear Science and Technology Organisation

The austenite to martensitic transformation and phase strain evolution under uniaxial tensile loading of Fe-Mn-3C-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: David Leonard1; Jean-Charles Stinville2; McLean Echlin3; Tresa Pollock4; 1University 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 Naragani1; Michael Sangid2; Paul Shade3; Jay Schuren4; Hemant Sharma5; Jun-Sang Park6; Peter Keneesi7; Joel Bernier8; Todd Turner9; 1Purdue University; 2Air Force Research Laboratory; 3Argonne National Laboratory; 4Lawrence 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 to characterize the microstructure. The centroid position, average orientation and stress state of the grains have been determined intermittently to characterize the microstructure.

11:20 AM
Investigation of Neighborhood Effects on Crack Initiation Sites in Different Ti Microstructures: Vahid Tar1; Michael Groeber2; Adam Pilchak3; Anthony Rollett4; 1Carnegie Mellon University; 2Air 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
Intragrann Orientation Spread Induced by Grain Interaction: Jette Oddershede1; Grethe Winther2; 1DTU Physics; 2DTU 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 Paradajape1; Partha Paul2; Jun-Sang Park3; Hemant Sharma4; Aaron Stebner5; L. Catherine Brinson6; 1Colorado School of Mines; 2Northwestern University; 3Argonne 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  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 Ferry1; 1University 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 Ulich1; Michael Grober1; J. Michael Scott1; 1Air Force Research Laboratory; 1UES, 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 Levinson1; David Rowenhorst1; 1Naval 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 microtomography 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 Echlin1; Jason Douglas1; William Lenth1; Ram Seshadri1; Tresa Pollock1; 1UC 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 length-scales 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 conductivity. Femtosecond laser based tomographic data has been gathered 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.

3:30 PM
Dictionary-Based Approach to Indexing of Electron Channeling Patterns: Saransh Singh1; Marc De Gare1; 1Carnegie 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
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. Furthermore, 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 Ziehmer1; Kaixiong Hu1; Ke Wang2; Erica
Lilleoedden1; 1Helmholtz-Zentrum Geesthacht; 2Technische 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 Choudhury1; 1Indian 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
July 12, 2016
Room: Salon III
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 Kaira1; Sudhanshu Singh1; Vincent De Andrade2; Francesco De
Carlo2; Nikhilesh Chawla3; 1Arizona State University; 2Advanced 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
Grains:
5:30 PM

locations with the overall distribution. normals calculated directly from the voxelized image using first order Cartesian like stress and strain, we also consider morphological influence using surface
The model produces full-field solutions for the stress and strain in voxelized a Fast-Fourier Transform-based elasto-viscoplastic (EVPFFT) formulation. deformed sample with micromechanical values obtained using a model with
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 differences will be correlated with the actual local environment of similar orientations are also observed, suggesting an effect of grain interactions. but differing somewhat from both of these. Some variations between grains of 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. Quantitative 3D Mapping of Local Stresses Near Dislocation Channel-Grain Boundary Interaction Sites in Irradiated Stainless Steel

Grains: Nicolai Judd1; Grethe Winther1; Jette Oddershede1; 1Technical 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.

5:30 PM

Measured Resolved Shear Stresses on Slip Systems in Austenitic Steel
Grains: Nicolai Judd1; Grethe Winther1; Jette Oddershede1; 1Technical 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

Multi-Modal Fusion of Experimental and Simulated Materials Data: Sean Donegan1; Mike Groeber2; Mike Uchic2; Adam Pilehak2; Dennis Dimiduk1; BlueQuartz Software; 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.

6:30 AM

Advances in Reconstruction Algorithms: Interface Quantification and the Registry of Multi-Modal Data
Wednesday AM
Room: Salon III
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 Rowenhorst1; 1The 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 Donegan1; Mike Groeber2; Mike Uchic2; Adam Pilehak2; Dennis Dimiduk1; BlueQuartz Software; 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.
Advances in 3D Materials Modeling: In-situ Experiments and Phase Field Simulations

Wednesday AM  Room: Salon IV  Location: Pheasant Run Resort
Session Chair: Henning Poulsen, Risoe DTU

8:00 AM Invited
In Situ Experiments in X Ray Tomography: Eric Maire1; ‘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 acquisition. 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 Sun1; Ahmed Cecen2; K. Aditya Mohan1; Xianghui Xiao1; Peter Voorhees3; ’Northwestern University; 2Georgia Institute of Technology; 3Purdue University; ’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 Yamanaka1; Kevin McReynolds2; Peter Voorhees3; ’Tokyo University of Agriculture and Technology; 2Northwestern 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 Rahnama1; Richard Dashwood1; Sridhar Seetharaman2; ’University of Warwick

A 3D phase field model was developed to simulate the evolution of ordered intermetallic compounds in multi-component Fe-C-Mo-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  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 Holm1; Brian DeCost2; ’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

TECHNICAL PROGRAM
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; Philip Withers; ‘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; Saransh Singh; Stefan Zaefferer; Tom Jäpel; Marc De Graef; ‘Carnegie Mellon University; ‘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; Jacob Jensen; Daniel Huber; Hamish Fraser; ‘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: (i) 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; Charudatta Phatak; Doga Gursoy; Francesco De Carlo; Vincent De Andrade; Begum Gulsoy; ‘Argonne National Laboratory; ‘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
10:30 AM
Dynamic In Situ Loading of Materials during Synchrotron 3D Tomographic Imaging: Brian Patterson1; Nikhilesh Chawla2; Sudhanshu Singh3; Angel Overjero4; Jason Williams5; Xianghui Xiao6; Kevin Henderson1; Robin Pacheco1; Nikolaus Cordes1; James Mertens1; 1Los Alamos National Laboratory; 2Arizona State University; 3Argonne 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 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 Décérot1; Jean-Yves Buffière1; vincent Maurel1; Fabien Szymtyka1; Alain Koster2; 1INSA de Lyon; 2MINES ParisTech; 3PSA Peugeot Citroen

The aim of this work is to study the initiation and propagation of cracks in a Lost Foam cast AlSiCuMg 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 realistic 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 particles 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, Crystal Plasticity Simulation and Machine Learning Technique: Andrea Rovinelli1; Michael Sangid2; Ricardo Lebiedbrishhti2; Wolfgang Ludwig1; Yoann Guilhelm1; Jean-Yves Buffière1; Vincent Maurel1; 1RWTH Aachen University; 2POSCO; 3Jülich Research Centre

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, Guilhelm, 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 Liu1; Sihwa Sung1; Deok-Chan Ahn1; Dong-Chul Chae1; Sebastian Münstermann1; Wolfgang Bleck1; 1RWTH Aachen University; 2POSTC; 3Jülich 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 Garcea1; Philip Withers2; 1The 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 held 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
July 13, 2016
Room: Salon III
Location: Pheasant Run Resort
Session Chair: Dorte Jensen, DTU Risø

2:00 PM Invited
MultiBeam Tomography: Current and Future Capabilities: Tresa Pollock1; William Lenthe2; McLean Echlin2; 1University of California Santa Barbara

The current capabilities of femtosecond lasers, in combination with focused ion beams, for generation of nm-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 Merkle1; Nikhilesh Chawla2; Sudhanshu Singh3; Lorenz Lechner4; 1Carl Zeiss X-ray Microscopy; 2Arizona State University

Here we detail a multi-scale tomographic study on an aluminum 7075 alloy, containing precipitates and inclusions, which has benefited from characterization of the same sample volume across multiple length scales and the subsequent quantification and analysis (shape, size, etc.). An efficient 3D correlation workflow topology 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 Shade1; Todd Turner1; Jay Schuren1; Basil Blank1; Joel Bernier1; Shiu Fai Li1; Jonathan Lind1; David Menasche1; Robert Suter1; Ulrich Lienert1; Peter Kenevel1; Jun-Sang Park1; Jonathan Almer2; Darren Dale; 
Ernest Fontes3; Matthew Miller4; ‘Air Force Research Laboratory’; 5PulseRay; 
6Lawrence Livermore National Laboratory; 7Carnegie Mellon University; 
8DESY; 9Advanced Photon Source; 10Cornell High Energy Synchrotron Source; 11Cornell 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 within 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

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
Éric Maire, Mateis Universite Lyon INSA
Dennis Dimiduk, Blue Quartz Software, LLC
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HOTEL FLOORPLANS

PHEASANT RUN RESORT

Mega Center

St. Charles Ballroom

3 - 4

Marsalis Ballroom

5 - 6

Broadway Ballroom

7 - 8

Amphitheater

9 - 10

Tower Penthouse Suites

11 - 12

Gem Rooms

13 - 14

Legends Rooms

15 - 16

Preservation Hall & Golf Meeting Rooms

17 - 18

New Orleans Ballroom

19 - 20

Bi-Level Suites

21 - 22

Golf Meeting Rooms

23 - 26

Courtyard Guest Rooms

Gallery Hall

Detailed information located on noted page numbers

PHEASANT RUN RESORT MAP

Mega Center

1 - 2

Bi-Level Suites

5 - 6

Business Center

9 - 10

Amphitheater

7 - 8

New Orleans Ballroom

17 - 18

Legends Rooms

13 - 14

Golf Meeting Rooms

23 - 26

Courtyard Guest Rooms

Gallery Hall

Detailed information located on noted page numbers

HOTEL FLOORPLANS
New Orleans Ballroom & Preservation Hall

New Orleans Ballroom features a soaring 20-foot ceiling, an historic long bar, a large built-in stage with an automated curtain and screen, adjustable incandescent and theatrical lighting and beautiful décor, which all blend together to make this an excellent choice for your next meeting or banquet.

For a more intimate environment, hold your event in one of our Preservation Hall rooms. These rooms offer space from over 630 to 1,630 square feet, have 10-foot ceilings, beautiful hardwood floors, a stage and adjustable lighting.

New Orleans Ballroom & Preservation Hall

<table>
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<th>Reception</th>
<th>Classroom</th>
<th>Theater</th>
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Notes:
MAKE YOUR PLANS FOR THE TMS 2017 ANNUAL MEETING & EXHIBITION!

Join your colleagues from nearly 70 nations at the meeting that the global minerals, metals, and materials community calls home.

More than 65 symposia are planned, including six symposia in the Computational Materials Science technical track:

- Computational Approaches to Materials for Energy Applications
- Computational Materials Discovery and Optimization – From Bulk to Materials Interfaces and 2D Materials
- Computational Methods and Experimental Approaches for Uncertainty Quantification and Propagation, Model Validation, and Stochastic Predictions
- Computational Thermodynamics and Kinetics
- ICME Gap Analysis: Structural Materials for Automotive Applications
- Materials by Design: An MPMD Symposium Honoring Greg Olson on the Occasion of His 70th Birthday

TMS2017 will also welcome two co-located international conferences, both included with your TMS2017 registration: 3rd Pan American Materials Congress and Energy Materials 2017. This year’s meeting will also feature the return of the popular student Bladesmithing Competition as part of the TMS2017 Exhibition.

Key TMS2017 Dates to Remember

- July 15, 2016: Final Deadline to Submit Abstracts
- September 1, 2016: Manuscripts Due for Proceedings
- October 2016: Registration Opens

Learn more at www.tms.org/TMS2017