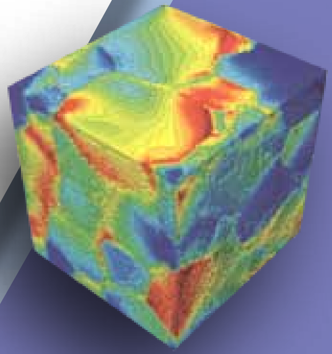
1st International Conference on

3DMS

3D Materials Science, 2012



FINAL PROGRAM

July 8-12, 2012 • Seven Springs Mountain Resort
Seven Springs, Pennsylvania, USA

ORGANIZED BY:

Alexis Lewis, Marc De Graef, Henning Friis Poulsen,
Jeff Simmons, and George Spanos

1st International Conference on 3DMS

3D Materials Science, 2012

SCHEDULE AT-A-GLANCE

Sunday, July 8

7:30 PM	*Plenary Session*
8:25 PM	Welcome Reception

Monday, July 9

8:15 AM	*Session 1: Applications of 3D Experimental Techniques Across Length Scales*	
10:15 AM	Discussion	
10:30 AM	Break	
10:45 AM	*Session 2: Applications of 3D Experimental Techniques Across Length Scales: Destructive Techniques*	*Session 3: Applications of 3D Experimental Techniques Across Length Scales: Structure-Property Relationships*
11:45 AM	Coffee Break	
12:00 PM	Session 2 (cont.)	Session 3 (cont.)
12:40 PM	Free Time	
4:00 PM	*Poster Session 1: 3D Interfaces, Microstructural Evolution, Structure-Property Relationships*	
5:30 PM	Free Time	
6:30 PM	*Session 4: Image Processing of 2D and 3D Microstructural Data*	
7:30 PM	Discussion	
7:45 PM	Session 4 (cont.)	
8:25 PM	Coffee Break	
8:45 PM	Session 4 (cont.)	
10:05 PM	Social Hour	

Tuesday, July 10

8:15 AM	*Session 5: Microstructure-Property Relationships in 3D*	
9:15 AM	Discussion	
9:30 AM	Break	
9:45 AM	*Session 6: Microstructure-Property Relationships in 3D: Fatigue, Failure and Deformation*	*Session 7: Microstructure-Property Relationships in 3D: Characterization and Simulation*
11:05 AM	Coffee Break	
11:20 AM	Session 6 (cont.)	Session 7 (cont.)
12:20 PM	Free Time	
4:00 PM	*Poster Session 2: Image Processing, Digital Representations of 3D Microstructures, and Applications of 3D Experimental Techniques*	
5:30 PM	Free Time	
6:30 PM	*Session 8: Digital Representation of 3D Microstructures*	
7:30 PM	Discussion	
7:45 PM	Session 8 (cont.)	
8:25 PM	Coffee Break	
8:45 PM	Session 8 (cont.)	
10:05 PM	Social Hour	

Wednesday, July 11

8:15 AM	*Session 9: 3D Interfaces and Microstructural Evolution*	
9:45 AM	Discussion	
10:00 AM	Break	
10:15 AM	*Session 10: 3D Interfaces and Microstructural Evolution: Boundaries and Grain Growth*	*Session 11: 3D Interfaces and Microstructural Evolution: Structure and Morphology*
11:15 AM	Coffee Break	
11:30 AM	Session 10 (cont.)	Session 11 (cont.)
12:30 PM	Free Time	
3:30 PM	*Student Poster Session*	
4:30 PM	Conference BBQ	
6:30 PM	*Session 12: Applications of 3D Experimental Techniques Across Length Scales: Non-Destructive Techniques*	
7:30 PM	Discussion	
7:45 PM	Session 12 (cont.)	
8:25 PM	Coffee Break	
8:45 PM	Session 12 (cont.)	
10:05 PM	Social Hour	

Thursday, July 12

8:15 AM	*Session 13: Future Directions in 3D Materials Science*
9:45 AM	Coffee Break
10:00 AM	Session 13 (cont.)
11:30 AM	Panel Discussion

Table of Contents

Welcome to the

1st International Conference on 3DMS

3D Materials Science, 2012

On behalf of The Minerals, Metals & Materials Society (TMS) and the conference organizers, I am pleased to welcome you to this premier event. The field of 3D materials science encompasses a broad range of research topics, and we have assembled experts in 3D data collection and analysis, image and data processing, modeling, and simulation, to exchange ideas, share new techniques and results, and move the field forward through collaborative efforts. I hope you will take every opportunity this week to discover the latest breakthroughs, learn about recent results, engage in the active exchange of ideas, and network with your fellow scientists, engineers, managers and students.

We look forward to an exciting meeting of dynamic discussions, outstanding speakers and interactive poster sessions, and we thank you for your participation in 3DMS 2012!

Warmest regards on behalf of the 3DMS 2012 Organizing Committee,
Alexis Lewis, U.S. Naval Research Laboratory

Organizing Committee:

Alexis Lewis	U.S. Naval Research Laboratory, USA
Marc De Graef	Carnegie Mellon University, USA
Henning Friis Poulsen	Risø National Laboratory and DTU, Denmark
Jeff Simmons	U.S. Air Force Research Laboratory, USA
George Spanos	The Minerals, Metals & Materials Society, USA

International Advisory Committee:

Dominique Bernard	ICMCB - Pessac, France
Charles Bouman	Purdue University, USA
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Larry Drummy	Air Force Research Laboratory, USA
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David Seidman	Northwestern University, USA
Gary Shiflet	University of Virginia, USA
Marco Stampanoni	ETH Zurich, Switzerland
Philip Withers	University of Manchester, UK

About the Conference

Registration

Your full-conference registration includes one copy of the proceedings disk. Your badge ensures admission to each of these events:

- Technical and Poster Sessions
- Access to the Exhibition
- Sunday Welcome Reception
- Monday, Tuesday, and Wednesday Social Hour
- Wednesday Barbecue

Registration Hours

The registration desk will be located in Stag Pass.

Sunday	5 to 9 p.m.
Monday	7:30 a.m. to 12:30 p.m. 4 to 6:30 p.m.
Tuesday	7:30 a.m. to 12:30 p.m. 4 to 6:30 p.m.
Wednesday	7:30 a.m. to 12:30 p.m. 3:30 to 6:30 p.m.
Thursday	7:30 to 11:30 a.m.

Technical Sessions

All oral presentations will be held in the Exhibit Hall or Sunburst Forum of Seven Springs Mountain Resort. Interactive discussions will follow invited presentations during each session. All poster presentations will be held in the Exhibit Hall. See the Technical Program section on pages 8-16 for room locations.

Proceedings

Full-conference registrants receive one copy of the proceedings as part of the registration fee. Additional copies may be purchased for $99.95 at www.wiley.com (TMS members receive a 25% discount). Approximately six weeks after the meeting, individual papers will be available through the Wiley Online Library: http://onlinelibrary.wiley.com.

Wi Fi

Complimentary internet access is available for 3DMS attendees in the hotel and meeting rooms.

Visit the TMS 3D Materials Repository and Materials Cyberinfrastructure Portal Booth!

Upload your 3D experimental and simulations data to the **3D Materials Atlas** and access online materials innovation tools and databases at the **Materials Cyberinfrastructure Portal**! TMS staff will be on hand to assist you with both of these valuable resources that offer the support you need to effectively interact with other researchers on 3D data sets, and implement materials and manufacturing innovation approaches and concepts.

Exhibit Information

Exhibition Hours

The exhibition will be located in the Exhibit Hall.

Sunday	7:30 to 8:30 p.m.
Monday	8 a.m. to 12:30 p.m. 4 to 5:30 p.m.
Tuesday	8 a.m. to 12:30 p.m. 4 to 5:30 p.m.
Wednesday	8 a.m. to 12:30 p.m. 3:30 to 4:30 p.m.

Exhibiting Companies (as of 6/19/12)

Clark – MXR, Inc.
FEI
Micro Photonics, Inc.
Scanco USA, Inc.
Simpleware
The Minerals, Metals & Materials Society (TMS)
UES, Inc.
Visualization Sciences Group (VSG)

Sunday set-up	5 to 7 p.m.
Wednesday dismantle	4:30 to 6:30 p.m.

Networking & Social Events

Welcome Reception

The Welcome Reception will be held on Sunday, July 8 from 8:25 to 9:25 p.m. in the Grand Ballroom.

Conference Barbecue

The barbecue will be held on Wednesday, July 11 from 4:30 to 6:30 p.m. at the Ski Lodge.

Social Hour

A social hour is planned each night (Monday-Wednesday) from 10:05 to 11:05 p.m. following the technical sessions in the Exhibit Hall. Don't miss this great networking opportunity!

Policies

Badges

All attendees must wear registration badges at all times during the conference 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 7, 2012. No refunds will be issued at the conference. Fees and tickets are nonrefundable.

Photography Notice

By registering for this conference, all attendees acknowledge that they may be photographed by conference personnel while at events and that those photos may be used for promotional purposes.

Audio/Video Recording Policy

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.

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 or PDAs on "silent" while in meeting rooms.

Recycling

Discard badges and programs in the bins located in the registration area.

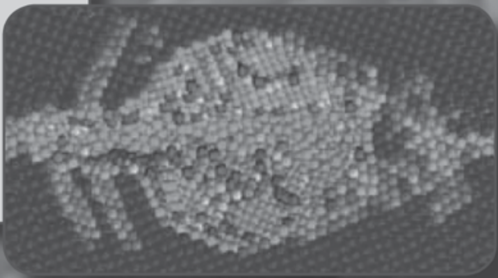
ABOUT THE VENUE

The Seven Springs Mountain Resort offers a multitude of on-site activities including a 6,685-yard, 18-hole golf course, as well as a tennis center, volleyball area, year-round swimming pool, exercise room, racquetball courts, bowling lanes, indoor miniature golf, family recreation center with video games, and numerous hiking trails surrounding the resort. Additional fees may apply. For more information visit www.7springs.com.

Seven Springs is located approximately one hour southeast of Pittsburgh. It is easily accessible off exits 91 or 110 of the Pennsylvania Turnpike. Pittsburgh International Airport is the nearest metropolitan terminal. Pickup from this airport is available by prior arrangement.

Taxi Service

Taxi service is available in the Greater Pittsburgh area. The area's two largest cab companies are Yellow Cab (412-665-8100) and People's Cab (412-681-3131). Cabs in Pittsburgh generally require a phone call to arrange for a pickup. Cabs are also available at the Pittsburgh International Airport.



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TECHNICAL SESSION LISTING

Sunday, July 8, 2012

Plenary Session Room: Exhibit Hall	
7:30 PM	**Introductory Comments**
7:35 PM	**Plenary**: **Perspectives on Materials Science in 3D**: *Dorte Jensen*[1]; [1]DTU Risø

Monday, July 9, 2012

Session 1: Applications of 3D Experimental Techniques Across Length Scales Room: Exhibit Hall	
8:15 AM	**Invited**: **Development of Multi-modal 3D Characterization Systems to Quantify Grain & Precipitate Microstructural Features in Aerospace Alloys**: *Michael Uchic*[1]; Michael Groeber[1]; Megna Shah[2]; Patrick Callahan[1]; Adam Shiveley[3]; Michael Chapman[3]; [1]Air Force Research Laboratory; [2]UES, Inc.; [3]SOCHE
8:45 AM	**Invited**: **Three-dimensional Characterization of Dislocation-Defect Interactions**: *Ian Robertson*[1]; Josh Kacher[1]; [1]University of Illinois at Urbana-Champaign
9:15 AM	**Invited**: **Acquisition of 3D Datasets for Property Prediction**: *Tresa Pollock*[1]; McLean Echlin[1]; Alessandro Mottura[1]; Chris Torbet[1]; [1]University of California Santa Barbara
9:45 AM	**Invited: Connecting Atomic Scale Crystallography and Chemistry through Atom Probe Tomography**: *Peter Felfer*[1]; Julie Cairney[1]; Vicente Araullo-Peters[1]; Saritha Simundrala[1]; [1]University of Sydney
10:15 AM	**Question and Answer Period**
10:30 AM	**Break**

Session 2: Applications of 3D Experimental Techniques Across Length Scales: Destructive Techniques Room: Exhibit Hall	
10:45 AM	**3D Multi-scale Electron Microscopy for Nano-scale Carbide Mapping in a Tempered 9 Cr Martensitic Steel**: *Niven Monsegue*[1]; Xin Jin[2]; Nana Kwame Yamoah[1]; Jeff Hawk[3]; William Reynolds[1]; Ge Wang[1]; Mitsuhiro Murayama[1]; [1]Virginia Tech; [2]Tsinghua University; [3]U.S. Department of Energy
11:05 AM	**Combining Atom-probe Tomography with Focused-ion Beam Microscopy for Targeted 3D Materials Characterization with Sub-nanometer Resolution**: *Dieter Isheim*[1]; David Seidman[1]; [1]Northwestern University
11:25 AM	**3D Orientation Imaging with Transmission Electron Microscopy**: *Søren Schmidt*[1]; Haihua Liu[2]; Andy Godfrey[3]; Henning Poulsen[1]; Xiaoxu Huang[1]; [1]Risoe DTU, Technical University of Denmark; [2]California Institute of Technology; [3]Tsinghua University
11:45 AM	**Break**
12:00 PM	**Electron Tomography in Aberration-corrected Transmission Electron Microscopes**: *Peter Ercius*[1]; [1]National Center for Electron Microscopy
12:20 PM	**FIB/SEM Determination of Sub-surface Damage Caused by Micro-tribology Scratching of WC/Co Hardmetal Samples**: *Mark Gee*[1]; Ken Mingard[1]; Andrew Gant[1]; Helen Jones[1]; [1]National Physical Laboratory

Session 3: Applications of 3D Experimental Techniques Across Length Scales: Structure-Property Relationships Room: Sunburst	
10:45 AM	**Atom-probe Tomography and the Science of a New Class of High-temperature Al-Sc Based Alloys**: *David Seidman*[1]; David Dunand[1]; [1]Northwestern University
11:05 AM	**3D Investigation of Cracking Behavior in a Ni Superalloy**: *Andrew Deal*[1]; David Rowenhorst[2]; Brandon Laflen[1]; Ian Spinelli[1]; Anthony Barbuto[1]; Yuchi Huang[1]; Timothy Hanlon[1]; [1]GE Global Research; [2]Naval Research Laboratory
11:25 AM	**Building Three Dimensional Microstructure of AA5754 Aluminum Sheet for Formability Simulation**: *Jonathan Rossiter*[1]; Kaan Inal[1]; Raja Mishra[2]; [1]University of Waterloo; [2]General Motors R&D
11:45 AM	**Break**
12:00 PM	**The TriBeam System: Femtosecond Laser Based Serial Sectioning**: *McLean Echlin*[1]; Alessandro Mottura[1]; Tresa Pollock[1]; [1]UC Santa Barbara

12:20 PM	**Characterization and Modeling Via Three-dimensional Reconstructions of Laser Welds in Stainless Steel**: *Jonathan Madison*[1]; [1]Sandia National Laboratories

4:00-5:30 PM	**Poster Session 1: 3D Interfaces, Microstructural Evolution, Structure-Property Relationships** **Room: Exhibit Hall**

P1-01: 3D Analysis of Surface Blisters, Subsurface Bubbles, and Underlying Microstructures of Implanted Metals: *John Smugeresky*[1]; Dan Huber[2]; Robert Kolasinski[1]; Don Cowgill[1]; John Sosa[2]; Hamish Fraser[2]; [1]Sandia National Laboratories, CA; [2]Ohio State University

P1-02: 3D Characterization of Recrystallization Boundaries: *Yubin Zhang*[1]; Dorte Juul Jensen[1]; [1]Danish-Chinese Center for Nanometals, Materials Research Division, Risø National Laboratory for Sustainable Energy, Technical University of Denmark

P1-03: 3D Microstructural Architectures for Metal and Alloy Components Fabricated by 3D Printing/Additive Manufacturing Technologies: *E. Martinez*[1]; L. E. Murr[1]; K. Amato[1]; J. Hernandez[1]; P. Shindo[1]; S. Gaytan[1]; D. Ramirez[1]; F. Medina[2]; R. Wicker[2]; [1]University of Texas at El Paso, Metallurgical and Materials Engineering; [2]University of Texas at El Paso, W. M. Keck Center for 3D Innovation

P1-04: 3D Microstructural Characterization of Uranium Oxide as a Surrogate Nuclear Fuel: Effect of Oxygen Stoichiometry on Grain Boundary Distributions: Karin Rudman[1]; Patricia Dickerson[2]; Darrin Byler[2]; Robert Dickerson[2]; Harn Lim[1]; Robert McDonald[1]; *Pedro Peralta*[1]; Kenneth McClellan[2]; [1]Arizona State University; [2]Los Alamos National Laboratory

P1-05: A Three-dimensional EBSD Investigation on the Distribution of Recrystallization Embryo in the Grain Boundary Regions of a Cold Rolled Low Carbon Steel: *Nasima Afrin*[1]; Md Zakaria Quadir[1]; Michael Ferry[1]; [1]University of New South Wales

P1-06: A Toolbox for Geometric Grain Boundary Characterization: *Krzysztof Glowinski*[1]; Adam Morawiec[1]; [1]Institute of Metallurgy and Materials Science, Polish Academy of Sciences

P1-07: An EBSD-based Characterization of Fe-9Ni and Fe-12Mn Martensitic Steels: *Christopher Kinney*[1]; Ken Pytlewski[1]; Y. Adachi[2]; J.W. Morris[1]; [1]University of California, Berkeley; [2]Kagoshima University

P1-08: Bainitic Microstructures in Weld Heat Affected Zones Studied by Electron Back-Scattering Diffraction: Joacim Hagström[1]; Bevis Hutchinson[1]; Oskar Karlsson[1]; Philip Withers[2]; *Ali Gholinia*[2]; [1]SwereaKIMAB AB; [2]The University of Manchester

P1-09: Atomic Density Function 3D Modeling of Crystal Growth with Different Symmetry: *Helena Zapolsky*[1]; Armen Khachaturyan[1]; Renaud Patte[1]; [1]University of Rouen

P1-10: Computing Fatigue Properties of Polycrystalline Ni-based Superalloy Microstructures using an Image-based Computational Approach: *Bin Wen*[1]; Nicholas Zabaras[1]; [1]Materials Process Design and Control Laboratory

P1-11: Effect of Grain Boundary Properties on Evolution of Lattice Orientations: *Jaehyung Cho*[1]; Chang-Seok Oh[1]; [1]Korea Institute of Materials Science

P1-12: Elastic Behavior of the Percolating Eutectic Structure of a High Pressure Die Cast Magnesium Alloy: *Bao Zhang*[1]; Anumalasetty Nagasekhar[1]; Carlos Caceres[1]; [1]The University of Queensland

P1-13: Fragmentation of a Steel Ring under Explosive Loading: *Jeremy Schreiber*[1]; Ivi Smid[1]; Timothy Eden[1]; [1]Penn State

P1-14: Gas Fast Reactors Fuel Claddings: Braids Densification Simulations and Equivalent Thermal Conductivities Calculations: *Sylvain Chupin*[1]; Patrick David[1]; Denis Rochais[1]; Francois Guillet[1]; Laurent Chaffron[2]; [1]CEA-Le Ripault; [2]CEA-Saclay

P1-15: Gating System Optimisation Design Study of a Cast Automobile Component Made in Aluminium Alloy: *Eyitayo Olakanmi*[1]; [1]Federal University of Technology

P1-16: Grain Boundary Networks in Polycrystalline Materials: Understanding Structure/Property Relationships: *Alexis Lewis*[1]; Andrew Geltmacher[1]; Siddiq Qidwai[1]; [1]Naval Research Laboratory

P1-17: In-situ Investigation of Damage and Strain Mechanisms in Structural Sheet Material via Synchrotron Radiation Laminography: Thilo Morgeneyer[1]; Lukas Helfen[2]; Francois Hild[3]; *Henry Proudhon*[1]; Ian Sinclair[4]; [1]Mines Paristech; [2]KIT; [3]ENS Cachan; [4]University of Southampton

P1-18: CANCELLED: K-phase in Fe-Al-Mn-C Alloys: Morphologies and Crystallographic Aspects: *Ian Zuazo*[1]; Helio Goldenstein[2]; Yves Bréchet[3]; Cyril Cayron[4]; [1]ArcelorMittal; [2]University of São Paulo; [3]SIMAP - Grenoble INP; [4]CEA-Grenoble, DRT/LITEN/DEHT/LCPEM

P1-19: Microstructural Analysis of MgB_2 Superconducting Wires by Electron Microscopy and X-ray Computed Tomography: Satoshi Hata[1]; *Yusuke Shimada*[1]; Masatoshi Mitsuhara[1]; Ken-ichi Ikeda[1]; Hideharu Nakashima[1]; Akiyoshi Matsumoto[2]; Kazumasa Togano[2]; Hiroaki Kumakura[2]; Hitoshi Kitaguchi[2]; Jung Ho Kim[3]; Shi Xue Dou[3]; Jeff Gelb[4]; Wenbing Yun[4]; [1]Kyushu University; [2]National Institute for Materials Science; [3]University of Wollongong; [4]Xradia Inc.

P1-20: Microstructure Visualization and Thermal Response Analysis of IF and Peritectic Mold Slag: *Pabitra Palai*[1]; Shainu Suresh[1]; T. K. Roy[1]; V. V. Mahashabde[1]; [1]Tata Steel Ltd., Jamshedpur, India

P1-21: Numerical Analysis and Experimental Study on Dry Friction and Wear Performance of SiC 3D Continuous Network Ceramic Reinforced Fe-40Cr Alloy: *Yu Liang*[1]; Jiang Yanli[1]; Senkai Lu[1]; Ru Hongqiang[1]; Ming Fang[1]; [1]Key Laboratory of New Processing Technology for Nonferrous Metals & Materials, Ministry of Education, College of Materials Science and Engineering

P1-22: Numerical Implementations of Crystal Plasticity in the Spectral Representation: *Bogdan Mihaila*[1]; Marko Knezevic[1]; Andres Cardenas[2]; [1]Los Alamos National Laboratory; [2]New York University

P1-23: Calculation of Lorentz Force Field of the Innovation Cathode Cell: *Jiang Yanli*[1]; Yu Liang[1]; Feng Naixiang[2]; [1]Key Laboratory of New Processing Technology for Nonferrous Metals & Materials, Ministry of Education, College of Materials Science and Engineering; [2]School of Materials and Metallurgy, Northeastern University

P1-24: Numerical Simulations of Compression Properties of SiC/Fe-20Cr Co-continuous Composites: *Yu Liang*[1]; Jiang Yanli[1]; Lu Senkai[1]; Ru Hongqiang[1]; Fang Ming[1]; [1]Key Laboratory of New Processing Technology for Nonferrous Metals & Materials, Ministry of Education, College of Materials Science and Engineering

P1-26: Parallel Potts Model for Recrystallization and Sintering: Sukbin Lee[1]; *Anthony Rollett*[1]; [1]Carnegie Mellon University

P1-27: State-of-the-art in Finite Element Modeling of Microstructural Descriptors: *Veera Sundararaghavan*[1]; Shang Sun[1]; Abhishek Kumar[1]; [1]University of Michigan

P1-28: Stress Relaxation in Polycrystals - Insights from Full-field Crystal Plasticity Fast Fourier Transform Approach: *Anand Kanjarla*[1]; Laurent Delannay[2]; Ricardo Lebensohn[1]; Huamiao Wang[3]; Carlos Tomé[1]; [1]Los Alamos National Laboratory; [2]Université Catholique de Louvain, Belgium; [3]McMaster University

P1-29: An Understanding of Embrittlement in Structural Materials Using 3D/4D Characterisation Methods: *Chiradeep Gupta*[1]; Hiroyuki Toda[1]; Masakazu Kobayashi[1]; Christian Schlacher[2]; Christof Sommitsch[2]; Peter Mayr[3]; Yoshio Suzuki[4]; Kentaro Useugi[4]; Akihisa Takeuchi[4]; [1]Toyohashi University of Technology; [2]Graz University of Technology; [3]Chemnitz University of Technology; [4]Japan Synchrotron Radiation Research Institute

P1-30: A Microscale Tension Test and Subsequent Serial Sectioning of an a+ß Titanium Alloy, Ti-6Al-2Sn-4Zr-6Mo: *Christopher Szczepanski*[1]; S.K. Jha[2]; R. Wheeler[3]; P.A. Shade[1]; J.M. Larsen[1]; [1]US Air Force Research Laboratory; [2]Universal Technology Corporation; [3]UES, Inc.

P1-31: Multi-scale Tomographic Analysis of Ductile Fracture in Ultrahigh Strength Steels: *Stephanie Chan*[1]; Dave Rowenhorst[2]; George Spanos[3]; Erik Lauridsen[4]; Wolfgang Ludwig[5]; Greg Olson[6]; [1]NextGen Aeronautics, Inc. ; [2]Naval Research Laboratory; [3]Currently The Minerals, Metals, and Materials Society; [4]Risø National Laboratory; [5]Laboratoire MATEIS; [6]Northwestern University

Session 4: Image Processing of 2D and 3D Microstructural Data
Room: Exhibit Hall

6:30 PM	**Invited: Shape Analysis and Classification of Objects**: *Brent Neal*[1]; John Russ[2]; [1]Milliken & Company; [2]North Carolina State University
7:00 PM	**Invited**: **Graph Cut Approaches for Materials Segmentation Preserving Shape, Appearance, and Topology**: Jarrell Waggoner[1]; Jeff Simmons[2]; Marc De Graef[3]; *Song Wang*[1]; [1]University of South Carolina; [2]Materials and Manufacturing Directorate, Air Force Research Labs; [3]Carnegie Mellon University
7:30 PM	**Question and Answer Period**
7:45 PM	**Simulation of FIB-SEM Images for Segmentation of Porous Microstructures**: *Torben Prill*[1]; Katja Schladitz[1]; Christian Wieser[2]; [1]Fraunhofer ITWM; [2]Adam Opel AG
8:05 PM	**A New Filtering Strategy for Noise Reduction on High Noise 3D Data Sets**: *Steven Van Boxel*[1]; Nghia Vo[2]; Peter Lee[1]; Philip Withers[1]; [1]University of Manchester; [2]Singapore Synchrotron Light Source
8:25 PM	**Break**
8:45 PM	**Microstructural Characterization of Porous Shape Memory Alloys using X-ray Tomography**: *David Rowenhorst*[1]; Catherine Tupper[2]; David Dunand[2]; [1]Naval Research Lab; [2]Northwestern University
9:05 PM	**Model Based HAADF STEM Tomography**: *Singanallur Venkatakrishnan*[1]; Lawrence Drummy[2]; Michael Jackson[3]; Marc Graef[4]; Charles Bouman[1]; Jeff Simmons[2]; [1]Purdue University; [2]AFRL; [3]BlueQuartz Software; [4]Carnegie Mellon University
9:25 PM	**Energy-based Segmentation Methods for Micrograph Analysis**: *Gunay Dogan*[1]; Stephen Langer[2]; Andrew Reid[2]; [1]Theiss Research; [2]National Institute of Standards and Technology
9:45 PM	**Generalized Forward Projectors for the Iterative Reconstruction of Electron Beam Serial Sectioning Data Sets**: *Marc De Graef*[1]; [1]Carnegie Mellon University

Tuesday, July 10, 2012

Session 5: Microstructure-Property Relationships in 3D
Room: Exhibit Hall

8:15 AM	**Invited**: **4D Materials Science: In-situ X-ray Synchrotron Tomography of Deformation in Metallic Materials**: *Nikhilesh Chawla*[1]; [1]Arizona State University
8:45 AM	**Invited**: **Combining X-ray Microtomography with Full Field Finite Elements Method to Study 3D Cracking in Stuctural Materials**: *Henry Proudhon*[1]; Jia Li[1]; Vincent Chiaruttini[2]; Thilo Morgeneyer[1]; Lucien Laiarinandrasana[1]; Samuel Forest[1]; Jean-Yves Buffière[3]; Wolfgang Ludwig[3]; [1]MINES ParisTech; [2]ONERA; [3]Université de Lyon
9:15 AM	**Question and Answer Period**
9:30 AM	**Break**

Session 6: Microstructure-Property Relationships in 3D: Fatigue, Failure and Deformation
Room: Exhibit Hall

9:45 AM	**3D Characterization and Modeling of Fatigue Cracks**: *Anthony Rollett*[1]; Clayton Stein[1]; Reeju Pokharel[1]; Jonathan Lind[1]; Joseph Tucker[1]; Albert Cerrone[1]; Anthony Ingraffea[1]; Robert Suter[1]; Peter Kenesei[2]; Ulrich Lienert[2]; [1]Carnegie Mellon University; [2]Advanced Photon Source (APS)
10:05 AM	**3D Characterization and Modeling of the Influence of Porosity on Fatigue Properties of a Cast Al Alloy**: *Jean-Yves Buffiere*[1]; Eric Maire[2]; Nicolas Vanderesse[3]; [1]Universite de Lyon INSA LYON ; [2]Universite de Lyon INSA LYON; [3]Ecole de Technologie Supérieure
10:25 AM	**In-situ Measurement of Lattice Strain in Al-Li Alloys**: *Armand Beaudoin*[1]; Mark Obstalecki[2]; Wesley Tayon[3]; Ulrich Lienert[4]; Peter Kenesei[4]; [1]University of Illinois at Urbana-Champaign; [2]Cornell University; [3]NASA; [4]Argonne National Laboratory
10:45 AM	**Numerical Simulation and Experimental Analysis of Notched Failure Processes in Composite Laminates**: *Ian Sinclair*[1]; Qingda Yang[2]; Mark Mavrogordato[1]; Brian Cox[3]; Mark Spearing[1]; [1]University of Southampton; [2]University of Miami; [3]Teledyne Scientific
11:05 AM	**Break**
11:20 AM	**3D Image-based Modeling of Residual Stresses in Hybrid Shape Memory Alloy / Ceramic Composites**: Brian Lester[1]; Yves Chemisky[1]; Dimitris Lagoudas[1]; Richard Everett[2]; Siddiq Qidwai[2]; *Andrew Geltmacher*[2]; [1]Texas A&M University; [2]Naval Research Laboratory
11:40 AM	**Integrated Experimental and Simulation Approaches for Mesoscopic Deformation of Polycrystalline Metal: Crystal Plasticity FEM**: *Yoon Suk Choi*[1]; Michael Groeber[2]; Paul Shade[2]; Todd Turner[2]; Jay Schuren[2]; Michael Uchic[2]; Christopher Woodward[2]; Dennis Dimiduk[2]; Triplicane Parthasarathy[1]; [1]UES, Inc.; [2]Air Force Research Lab.

Session 7: Microstructure-Property Relationships in 3D: Characterization and Simulation
Room: Sunburst

9:45 AM	**Twin Connectivity in Wrought Magnesium Alloys**: Matthew Barnett[1]; Alireza Ghaderi[1]; *Mark Nave*[1]; [1]Deakin University
10:05 AM	**CANCELLED: The Influence of 3D Networks of Aluminides on the Strength of Al-Si Piston Alloys**: *Guillermo Requena*[1]; Zahid Asghar[1]; [1]TU Vienna
10:25 AM	**Measurements of Materials During In-situ Experiments Using X-ray Tomography**: *Brian Patterson*[1]; Kevin Henderson[1]; Robert Gilbertson[1]; Christopher Hamilton[1]; Kimberly Obrey[1]; Nickolaus Smith[1]; [1]Los Alamos National Laboratory
10:45 AM	**Development of Fully Automated Serial-sectioning 3D Microscope and Topological Approach to Pearlite and Dual-phase Miscrostructure in Steels**: *Yoshitaka Adachi*[1]; Naoko Sato[1]; [1]Kagoshima University
11:05 AM	**Break**
11:20 AM	**Quantification of Primary Phase Undercooling of Rapidly Solidified Droplets with 3D Microtomography**: Arash Ilbagi[1]; Pooya Delshad Khatibi[1]; *Hani Henein*[1]; Charles-Andre Gandin[2]; Dieter Herlach[3]; [1]University of Alberta; [2]MINES ParisTech & CNRS, CEMEF UMR; [3]c/o Institute of Materials Physics in Space, DLR
11:40 AM	**Using Combined EBSD/EDS to Characterise Nickel-based Superalloys in 3D**: *Geoff West*[1]; Rachel Thomson[1]; Daniel Child[1]; [1]Loughborough University
12:00 PM	**The Influence of Microstructure on 3D Crack Morphologies in a New Naval Steel**: *Marie Cox*[1]; David Rowenhorst[2]; Richard Fonda[2]; [1]National Research Council Postdoctoral Fellow; [2]U.S. Naval Research Laboratory

4:00-5:30 PM	Poster Session 2: Image Processing, Digital Representations of 3D Microstructures, and Applications of 3D Experimental Techniques Room: Exhibit Hall

P2-01: 3D Characterization and Reconstruction of the Primary Austenite Dendrite and Interdendritic Space in Lamellar Cast Iron: *Attila Diószegi*[1]; Ruben Lora[1]; Vasilios Fourlakidis[2]; Guillem Prats Vilaseca[1]; Álvaro Díaz de Aguilar[1]; [1]Jönköping University; [2]Swerea Swecast AB

P2-02: 3D Characterization of Damage within Copper using Micro and Nano X-ray Tomography: *Brian Patterson*[1]; Kevin Henderson[1]; Ellen Cerreta[1]; J Escobedo-Diaz[1]; Darcie Dennis-Koller[1]; [1]Los Alamos National Laboratory

P2-03: 3D Characterization of High Burn-up MOX Fuel: *Melissa Teague*[1]; Jessica Riesterer[1]; Brian Gorman[1]; Michael Tonks[1]; [1]Idaho National Laboratory

P2-04: 3D Identification of Inclusions in NiTi Alloy after Electropolishing: *Tadeusz Hryniewicz*[1]; Ryszard Rokicki[1]; [1]Politechnika Koszalinska

P2-05: Advances in 3D Imaging and Analysis of Materials Using Electron and Ion Beams: *Hans Fleurkens*[1]; Daniel Phifer[1]; [1]FEI Company

P2-06: Automated Segmentation and Characterization of 2D/3D Fibrous Composite Optical Micrographs using the Hough Transform: *Craig Przybyla*[1]; [1]Air Force Research Laboratory

P2-07: Development of a Data Fusion Module to Register and Combine EBSD, EDS, and Electron-optic Images: *Megna Shah*[1]; Michael Uchic[2]; Michael Groeber[2]; [1]UES, Inc.; [2]Air Force Research Laboratory

P2-08: Digital Representation Environment for the Analysis of Microstructure in 3D (DREAM.3D): *Michael Groeber*[1]; Michael Jackson[2]; [1]AFRL; [2]BlueQuartz Software

P2-09: FIB/SEM Tomography as a Tool to Study Bulk Membrane Recycling in Central Synapses: *Liubov Belova*[1]; Oleg Shupliakov[2]; [1]KTH, Royal Institute of Technology; [2]Karolinska Institute

P2-10: 3D Analysis of Phase Separation in Ferritic Stainless Steels: Joakim Odqvist[1]; Jing Zhou[1]; Wei Xiong[1]; *Peter Hedström*[1]; Mattias Thuvander[2]; Malin Selleby[1]; John Ågren[1]; [1]KTH (Royal Institute of Technology); [2]Chalmers University of Technology

P2-11: Generation of Micro-Architectures: Philippe Young[1]; David Raymont[1]; Liang Hao[1]; *Kerim Genc*[2]; [1]University of Exeter; [2]Simpleware Ltd.

P2-12: Handling Misalignment and Drift in 3D EBSD Data Sets: Yuchi Huang[1]; *Brandon Laflen*[1]; Andrew Deal[1]; Ian Spinelli[1]; Anthony Barbuto[1]; Timothy Hanlon[1]; [1]GE Global Research

P2-13: High Energy Diffraction Microscopy as a Tool for High Pressure Research: *Joel Bernier*[1]; Nathan Barton[1]; Donald Boyce[2]; Daniel Farber[3]; [1]Lawrence Livermore National Laboratory, Engineering Technologies Division; [2]Cornell University, Sibley School of Mechanical and Aerospace Enginering; [3]Lawrence Livermore National Laboratory, Condensed Matter and Materials Division

P2-14: In-situ Investigations of the Interface Dynamics of Materials using Ultra-fast X-ray Tomographic Microscopy and Laser Heating: *Julie Fife*[1]; Peter Voorhees[2]; Marco Stampanoni[3]; [1]Paul Scherrer Institut; [2]Northwestern University; [3]Paul Scherrer Institut and ETH and University of Zurich

P2-15: In-situ Tomographic Imaging of 3D Microporous Composite Anode of Lithium-ion Batteries: *XIanghui Xiao*[1]; Fikile Brushett[1]; Lynn Trahey[1]; John Vaughey[1]; [1]Argonne National Laboratory

P2-16: Optimizing Scholastic Process for Efficient Microstructure Reconstruction: *Seun Ryu*[1]; Dongsheng Li[1]; [1]Pacific Northwest National Laboratory

P2-17: Investigating Shock Damage in Polycrystalline Cu through High-Energy Diffraction Microscopy: *John Bingert*[1]; R.M. Suter[2]; J. Lind[2]; S.F. Li[2]; C.M. Hefferan[2]; C.P. Trujillo[1]; [1]Los Alamos National Laboratory; [2]Carnegie Mellon University

P2-18: Investigation of the 3D Grain Size and Shape of WC in Cemented Carbides: *Ali Gholinia*[1]; Bartlomiej Winiarski[1]; Philip J. Withers[1]; Ida Borgh[2]; Peter Hedström[2]; Joakim Odqvist[2]; Annika Borgenstam[2]; Ken Mingard[3]; Mark G Gee[3]; [1]University of Manchester; [2]KTH Royal Institute of Technology; [3]National Physical Laboratory

P2-20: Micro-computed Tomography, a 3D Tool for Non-destructive Visualisation and Analysis: *Evi Bongaers*[1]; Remy Van den Bosch[2]; [1]SkyScan N.V.; [2]University of Antwerp

P2-21: Multi-scale Homogenisation for 3D Microstructures: Philippe Young[1]; David Raymont[1]; Liang Hao[1]; *Kerim Genc*[2]; [1]University of Exeter; [2]Simpleware Ltd.

P2-22: Study of Three Dimensional Microstructural Morphologies of Dendritically Solidified Alpha-Mg(X): *Mingyue Wang*[1]; Tao Jing[2]; [1]Tsinghua University & Arizona State University; [2]Tsinghua University

P2-23: Three Dimensional Composition Mapping of a White Spot VAR Defect in Nickel Alloy 718: *Trevor Watt*[1]; Eric Taleff[1]; [1]The University of Texas at Austin

P2-24: Three Dimensional Segmentation and Reconstruction from Serial Micrographs of Powder Metallurgy Polycrystals: *Michael Marsh*[1]; Laurent Bernard[2]; Murali Gorantla[3]; Yoon Suk Choi[3]; [1]Visualization Sciences Group; [2]Noesis; [3]UES

P2-25: Tracking Geometrical Features using Near-field High Energy X-ray Diffraction Microscopy: *S. F. Li*[1]; J. Lind[2]; C. M. Hefferan[2]; A. D. Rollett[2]; R. M. Suter[2]; [1]Lawrence Livermore National Lab; [2]Carnegie Mellon University

P2-26: X-ray Micro-Laue Diffraction in 3D at the Canadian Light Source: *Renfei Feng*[1]; [1]Canadian Light Source	
P2-27: Characterization of Carbonate Rocks through X-ray Microtomography: Debora Pilotto[1]; Sérgio da Fontoura[1]; *Sidnei Paciornik*[2]; Marcos Henrique Mauricio[1]; [1]PUC-Rio; [2] PUC-Rio	
P2-28: Characterization of Pores and Cracks in Underwater Welds by µCT and Digital Optical Microscopy: *Sidnei Paciornik*[1]; Timo Bernthaler[2]; Valter dos Santos[3]; Mauricio Monteiro[3]; Marcos Henrique Mauricio[3]; Alexandre Bracarense[4]; Ezequiel Pessoa[5]; [1] PUC-Rio; [2]Hochschule Aalen - Technik und Wirtschaft; [3]PUC-Rio; [4]UFMG; [5]CEFET-MG	

Session 8: Digital Representation of 3D Microstructures
Room: Exhibit Hall

6:30 PM	**Invited**: **Storage and Sharing of Large 3D Imaging Datasets**: Richard Boardman[1]; *Ian Sinclair*[1]; Simon Cox[1]; Philippa Reed[1]; Kenji Takeda[1]; Jeremy Frey[1]; Graeme Earl[1]; [1]University of Southampton
7:00 PM	**Invited**: **The State of 3D Synthetic Microstructure Generation and Its Novel Applications**: *Michael Groeber*[1]; Anthony Rollett[2]; Joseph Tucker[2]; Michael Jackson[3]; [1]AFRL; [2]Carnegie Mellon University; [3]BlueQuartz Software
7:30 PM	**Question and Answer Period**
7:45 PM	**Model Reduction and Reconstruction of Realistic Microstructures for Computing Property Variability**: *Nicholas Zabaras*[1]; Bin Wen[1]; [1]Materials Process Design and Control Laboratory
8:05 PM	**The OOF Project at NIST**: *Stephen Langer*[1]; Andrew Reid[1]; Günay Dogan[2]; [1]National Institute of Standards and Technology; [2]NIST/Theiss Research
8:25 PM	**Break**
8:45 PM	**Fitting Laguerre Tessellations to the Microstructure of Cellular Materials**: *Irene Vecchio*[1]; Katja Schladitz[1]; Claudia Redenbach[2]; [1]Fraunhofer ITWM; [2]University of Kaiserslautern
9:05 PM	**A Implicit Model for Generating Polycrtalline Structures and Unstructured Meshes**: *LiangXing Lv*[1]; Liang Zhen[1]; Wenzhu Shao[1]; [1]Harbin Institute of Technology
9:25 PM	**Stereology and 3D Grain Boundary Network Analysis**: *Bryan Reed*[1]; Brent Adams[2]; Joel Bernier[1]; Chris Hefferan[3]; Alisa Henrie[2]; Shiu Li[3]; Jonathan Lind[3]; Robert Suter[3]; Mukul Kumar[1]; [1]Lawrence Livermore National Laboratory; [2]Brigham Young University; [3]Carnegie Mellon University

Wednesday, July 11, 2012

Session 9: 3D Interfaces and Microstructural Evolution
Room: Exhibit Hall

8:15 AM	**Invited**: **Diffraction-based 3D Imaging of Microstructural Evolution**: *Erik Lauridsen*[1]; [1]Risø-DTU
8:45 AM	**Invited**: **Interfacial Morphology and Evolution in Solid-Liquid Mixtures**: J. Gibbs[1]; J. Fife[2]; *Peter Voorhees*[1]; [1]Northwestern University; [2]Swiss Light Source
9:15 AM	**Invited**: **3-dimensional Measurement and Description of the 5-parameter Grain and Phase Boundary Character in Steels**: Stefan Zaefferer[1]; *Peter Konijnenberg*[1]; [1]Max-Planck-Institute for Iron Research
9:45 AM	**Question and Answer Period**
10:00 AM	**Break**

Session 10: 3D Interfaces and Microstructural Evolution: Boundaries and Grain Growth
Room: Exhibit Hall

10:15 AM	**Quantitative Analysis of Three-dimensional Grain Growth**: Trevor Keller[1]; *Dan Lewis*[1]; [1]Rensselaer Polytechnic Institute
10:35 AM	**The Shapes of a 3D Grain Growth Microstructure**: *Emanuel Lazar*[1]; Jeremy Mason[2]; Robert MacPherson[1]; David Srolovitz[3]; [1]Institute for Advanced Study; [2]Lawrence Livermore National Laboratory; [3]Institute of High Performance Computing, A*Star
10:55 AM	**Topological Mechanism of Grain Growth**: *Burton Patterson*[1]; Robert DeHoff[1]; Veena Tikare[2]; Zhiwei Sun[3]; David Rule[1]; Amy Adams[1]; [1]University of Florida; [2]Sandia National Laboratory; [3]University of Alabama at Birmingham
11:15 AM	**Break**

11:30 AM	**Distribution of Carbide Particles and Its Influence on Grain Growth of Ferrite in Fe-C Alloys Containing B and V**: Takafumi Oikawa[1]; *Masato Enomoto*[1]; [1]Ibaraki University
11:50 AM	**Modeling Grain Boundary Interfaces in Pure Nickel**: *Todd Turner*[1]; Jay Schuren[1]; Paul Shade[1]; Michael Groeber[1]; [1]Air Force Research Laboratory
12:10 PM	**3D Stochastic Ginzburg-Landau Model of Non-Classical Nucleation**: *Alexander Umantsev*[1]; [1]Fayetteville State University

Session 11: 3D Interfaces and Microstructural Evolution: Structure and Morphology
Room: Sunburst

10:15 AM	**On the Three-dimensional Microstructure of Martensite in Carbon Steels**: *Peter Hedström*[1]; Albin Stormvinter[1]; Annika Borgenstam[1]; Ali Gholinia[2]; Bartlomiej Winiarski[2]; Philip J. Withers[2]; Oskar Karlsson[3]; Joacim Hagström[3]; [1]KTH - Royal Institute of Technology; [2]University of Manchester; [3]Swerea KIMAB AB
10:35 AM	**Morphology and Crystallography of Annealing Twins in Austenite**: *Milo Kral*[1]; Ben Gardiner[1]; [1]University of Canterbury
10:55 AM	**Three-dimensional Morphology Due to Phase Separation in an Fe-Ni-Al Alloy Studied by STEM Tomography**: *Syo Matsumura*[1]; Keisuke Ogata[1]; Satoshi Hata[1]; Minoru Doi[2]; Hideharu Nakashima[1]; [1]Kyushu University; [2]Aichi Insitute of Technology
11:15 AM	**Break**
11:30 AM	**3D Characterization of Microstructural Evolution in Anisotropic Ceramics**: *Melanie Syha*[1]; Wolfgang Rheinheimer[1]; Michael Bäurer[1]; Wolfgang Ludwig[2]; Erik Lauridsen[3]; Daniel Weygand[1]; Peter Gumbsch[1]; [1]Karlsruhe Institute of Technology; [2]European Synchrotron Radiation Facility; [3]Risø National Laboratory
11:50 AM	**Structural Evolution of Nanoporous Gold during Thermal Coarsening as Determined by X-ray Nano-tomography**: Yu-chen Chen[1]; Steve Wang[2]; Yong Chu[3]; Wenjun Liu[2]; Ian McNulty[2]; Peter Voorhees[4]; *David Dunand*[4]; [1]Northwestern University, Argonne National Lab.; [2]Argonne National Lab.; [3]Brookhaven National Lab.; [4]Northwestern University
12:10 PM	**Exploring 3D Interfaces and Microstructural Evolution with Micro-Laue Diffraction**: *Rozaliya Barabash*[1]; Jon Tischler[1]; John Budai[1]; Wenjun Liu[2]; [1]Oak Ridge National Laboratory; [2]Advanced Photon Source

3:30 - 4:30 PM — Student Poster Session
Room: Exhibit Hall

P3-01: 3D Visualisation of Crystallographic Pitting: *Alice Laferrere*[1]; Nick Parson[2]; Xiaorong Zhou[1]; George Thompson[1]; [1]The University of Manchester; [2]Rio Tinto Alcan

P3-02: 3D Analysis on the Effect of Creep Behavior on Phase Morphology of Duplex 2205 during the Continuous Annealing: *Heeyong Park*[1]; Bruno De Cooman[1]; [1]GIFT, POSTECH

P3-03: 3D Atom Probe Investigation of Nanoscale Austenite Reversion at Interfaces in a Martensitic Stainless Steel: *Lei Yuan*[1]; Dirk Ponge[1]; Dierk Raabe[1]; [1]Max-Planck-Institut fuer Eisenforschung

P3-04: 3D Microstructure Analysis in Macro-micro Scale: *Yeom Kyu Jung*[1]; Seong Bum Son[1]; Chan Soon Kang[1]; Jong Soo Cho[1]; Jeong Tak Moon[2]; Heung Nam Han[1]; Kyu Hwan Oh[1]; [1]Seoul National University; [2]MK Electron

P3-05: 3D Microstructure Construction of Sintered ZrO2 under Different Sintering Conditions: *Zhenbo Xia*[1]; Kathy Lu[1]; [1]Virginia Polytechnic Institute and State University

P3-06: 3D Microstructures of Sb_2Te_3 Precipitates in PbTe Matrix and Their Elongations with Prediction by a Weak Compatibility Condition: *Xian Chen*[1]; Shanshan Cao[2]; Teruyuki Ikeda[3]; Jeffrey Snyder[4]; Dominique Schryvers[5]; Richard James[1]; [1]University of Minnesota; [2]South China University of Technology; [3]PRESTO; [4]California Institute of Technology; [5]University of Antwerp

P3-07: Bulk Three-dimensional Magnetic Domain Structure in a Slightly Misoriented (110)[001] FeSi Single Crystal: Sunmi Shin[1]; Rudolf Schaefer[2]; *B. C. De Cooman*[1]; [1]Pohang University of Science and Technology; [2]IFW Dresden

P3-08: Calculation of Grain Boundary Character Distribution from Three Dimensional EBSD Data: *Hadi Pirgazi*[1]; Roumen Petrov[2]; Leo Kestens[1]; [1]Gent University; [2]Delft University of Technology

P3-09: Deformation Mechanisms Studied in Commercially Pure Titanium by Combined use of X-ray Diffraction Contrast Tomography (DCT) and Scanning Micro-diffraction Procedures: *Laura Nervo*[1]; Michael Preuss[2]; João Quinta da Fonseca[2]; Wolfgang Ludwig[3]; Andrew King[4]; [1]ESRF & University of Manchester; [2]University of Manchester; [3]INSA de Lyon; [4]ESRF

P3-10: Design of Virtual 3D Micostructures with Controlled Grain Size and Orientation Distribution: *Edgar de Araujo*[1]; K. Verbeken[1]; L.A.I. Kestens[1]; [1]Gent University

P3-11: Four-dimensional Characterization of Coarsening of Complex Microstructures via Phase-field Method: *Chal-Lan Park*[1]; Peter W. Voorhees[2]; Katsuyo Thornton[1]; [1]University of Michigan; [2]Northwestern University

P3-12: In-situ Characterization of Entrainment Defects in Liquid Al-Si-Mg Alloy: *Yang Yue*[1]; William Griffiths[1]; Julie Fife[2]; Nick Green[1]; [1]University of Birmingham, UK; [2]Swiss Light Source, PSI

P3-13: Influence of Serial Section Thickness on the Measurement Precision of 3D Grain Volume and Surface: *Binbin Zhang*[1]; Guoquan Liu[1]; [1]USTB

P3-14: Investigation of Creep Damage in Martensitic 9-12% Cr Steel using Synchrotron X-ray Micro-tomography: *Christian Schlacher*[1]; Peter Mayr[2]; Francisca Mendez Martin[3]; Chiradeep Gupta[4]; Hiroyuki Toda[4]; Kentaro Uesugi[5]; Yoshio Suzuki[5]; Christof Sommitsch[3]; [1]Graz University of Technology ; [2]Chemnitz University of Technology; [3]Graz University of Technology; [4]Toyohashi University of Technology; [5]Japan Synchrotron Radiation Research Institute

P3-15: Microstructure-based Life Modeling of Ni-based Superalloys: *Joseph Tucker*[1]; Albert Cerrone[2]; Anthony Rollett[1]; Anthony Ingraffea[2]; [1]Carnegie Mellon University; [2]Cornell University

P3-16: Microstructure Change of SOFC Anode during Long Term Operation using 3D Reconstruction: *Harshil Parikh*[1]; Arthur Heuer[1]; Mark De Guire[1]; Zhien Liu[2]; Richard Goettler[2]; [1]Case Western Reserve University; [2]Rolls-Royce Fuel Cell Systems (US) Inc.

P3-17: Modeling 3D Grain Coarsening Based on Tomography Data: *Melanie Syha*[1]; Daniel Weygand[1]; Peter Gumbsch[2]; [1]Karlsruhe Institute for Technology; [2]Karlsruhe Institute of Technology

P3-18: Novel 3D Characterization for the Advanced Understanding of Stereological Quantification of a+ß Titanium Alloys: *John Sosa*[1]; Daniel Huber[1]; Vikas Dixit[1]; Peter Collins[2]; Hamish Fraser[1]; [1]The Ohio State University; [2]University of North Texas

P3-19: Pitfalls in Direct 3D Characterization for Microstructural Quantification of a+ß Titanium Alloys: *Daniel Huber*[1]; John Sosa[1]; Margaret Noble[1]; Vikas Dixit[1]; Peter Collins[2]; Hamish Fraser[1]; [1]The Ohio State University; [2]University of North Texas

P3-20: Quantifying the Effect of Spatial Resolution on the Accuracy of 3D Feature Characterization: *Gregory Loughnane*[1]; Ramana Grandhi[1]; Raghavan Srinivasan[1]; Michael Uchic[2]; Michael Groeber[2]; Matthew Riley[3]; Megna Shah[4]; [1]Wright State University; [2]Air Force Research Laboratory; [3]University of Idaho; [4]UES, Inc.

P3-21: Quantitative Analysis and Comparison of γ Precipitate Shapes in a Series of Ni-based Superalloys: *Patrick Callahan*[1]; Marc De Graef[1]; [1]Carnegie Mellon University

P3-22: Reconstruction of γ Precipitate Shapes in Ni-base Superalloys by Means of 3D Zernike Functions: *Patrick Callahan*[1]; Marc De Graef[1]; [1]Carnegie Mellon University

P3-23: Representation in 3D and Stress Response of Tin Whiskers: *Benjamin Anglin*[1]; Pylin Sarobol[2]; Aaron Pedigo[2]; Wei-Hsun Chen[2]; Ricardo Lebensohn[3]; John Blendell[2]; Carol Handwerker[2]; Anthony Rollett[1]; [1]Carnegie Mellon University; [2]Purdue University; [3]Los Alamos National Laboratory

P3-24: SEM-based Electron Tomography of Turfs Comprised of Lineal Structures: *Osama Fakron*[1]; D.P. Field[1]; [1]WSU

P3-25: The Microstructure of RR1000 Nickel-base Superalloy: The FIB-SEM Dual-beam Approach: *Stephen Croxall*[1]; Mark Hardy[2]; Howard Stone[1]; Paul Midgley[1]; [1]University of Cambridge; [2]Rolls Royce plc

P3-26: The Time Evolution of Three Grains in a Thin Film: *Vadim Derkach*[1]; Amy Novick-Cohen[1]; Arcady Vilenkin[2]; [1]Technion-IIT; [2]Hebrew University

P3-27: Three-dimensional Atomic and Defect Structures of Ultra Thin Au and Au-alloy Nanowires: *Chun-Hsien Wu*[1]; Niven Monsegue[1]; William Reynolds[1]; Deborah Aruguete[2]; Michael Hochella[1]; Xin Jin[1]; Ge Wang[1]; Mitsuhiro Murayama[1]; [1]Virginia Tech; [2]National Science Foundation

P3-28: Three-dimensional Investigation of Void Growth Leading to Fracture in Commercially Pure Titanium: *Marina Pushkareva*[1]; Jérôme Adrien[2]; Eric Maire[2]; Arnaud Weck[1]; [1]University of Ottawa; [2]INSA de Lyon

P3-29: Three Dimensional Simulation of Dendritic Solidification by Lattice Boltzmann and Cellular Automaton Methods: *Mohsen Eshraghi*[1]; Sergio Felicelli[1]; [1]Mississippi State University

P3-30: Subgrain Boundary Identification in 3D EBSD Data through Fast Multiscale Clustering: *Brian Soe*[1]; Cullen McMahon[1]; David Golay[1]; Zakaria Quadir[2]; Michael Ferry[2]; Lori Bassman[1]; [1]Harvey Mudd College; [2]University of New South Wales

P3-31: Use of Serial Sectioning to Characterize Local Grain Boundary Structures in Nickel-Based Superalloys: *Jennifer L.W. Carter*, John M. Sosa[1], Paul A. Shade[2], Hamish L. Fraser[1], Michael D. Uchic[2], Michael J. Mills[1] ; [1] Department of Materials Science and Engineering, The Ohio State University; [2] Air Force Research Laboratory, Materials & Manufacturing Directorate, AFRL/RXLM, Wright Patterson AFB

Session 12: Applications of 3D Experimental Techniques Across Length Scales: Non-Destructive Techniques
Room: Exhibit Hall

6:30 PM	**Invited**: **Ultra Fast Tomography: New Developments for 4D Studies in Material Science**: *Pierre Lhuissier*[1]; Mario Scheel[2]; Marco Di Michiel[2]; Elodie Boller[2]; Jérôme Adrien[3]; Eric Maire[3]; Luc Salvo[1]; Jean-Jacques Blandin[1]; Michel Suery[1]; [1]SIMaP/GPM2-CNRS-Grenoble University; [2]ESRF; [3]MATEIS - INSA Lyon
7:00 PM	**Invited**: **High Energy X-ray Diffraction Microscopy Microstructure Mapping**: *Robert Suter*[1]; Shiu Fai Li[2]; Christopher Hefferan[1]; Jonathan Lind[1]; Reeju Pokharel[1]; Ulrich Lienert[3]; Anthony Rollett[1]; [1]Carnegie Mellon University; [2]Lawrence Livermore National Laboratory; [3]Argonne National Laboratory
7:30 PM	**Question and Answer Period**
7:45 PM	**High-speed Micro Imaging with Polychromatic Hard X-ray Synchrotron Radiation for Academic and Industrial Applications**: *Elodie Boller*[1]; Paul Tafforeau[1]; Alexander Rack[1]; Carmen Soriano[1]; Sophie Sanchez[1]; [1]ESRF
8:05 PM	**X-ray Dark Field Microscopy**: Henning Poulsen[1]; *Andrew King*[2]; Wolfgang Ludwig[2]; Anatoly Snigirev[2]; [1]Risoe DTU; [2]ESRF
8:25 PM	**Break**
8:45 PM	**CANCELLED: Characterization of Orientation and Elastic Strain Gradients Inside Bulk Grains by Means of X-ray Diffraction Imaging Techniques**: *Wolfgang Ludwig*[1]; Andrew King[2]; Peter Reischig[2]; Nicola Vigano[1]; Laura Nervo[2]; [1]Université de Lyon; [2]ESRF
9:05 PM	**Diffraction-Amalgamated Grain-Boundary Tracking (DAGT) Technique Applied to Al-3mass%Cu**: *Darren LeClere*[1]; Takanobu Kamiko[1]; Masakazu Kobayashi[1]; Kentaro Uesugi[2]; Akihisa Takeuchi[2]; Yoshio Suzuki[2]; Hiroyuki Toda[1]; [1]Toyohashi University of Technology; [2]Japan Synchrotron Radiation Research Institute
9:25 PM	**X-ray Tomographic Microscopy at TOMCAT: Resolving the Dynamics of Materials**: *Julie Fife*[1]; Rajmund Mokso[1]; Michel Rappaz[2]; Marco Stampanoni[3]; [1]Paul Scherrer Institut; [2]Ecole Polytechnique Fédérale de Lausanne; [3]Paul Scherrer Institut and ETH and University of Zurich
9:45 PM	**Measurement and Quantification of Grain Boundary Evolution in Three Dimensions during Grain Coarsening**: *S. F. Li*[1]; B. W. Reed[1]; J. V. Bernier[1]; C. M. Hefferan[2]; J. Lind[2]; R. M. Suter[2]; M. Kumar[1]; [1]Lawrence Livermore National Lab; [2]Carnegie Mellon University

Thursday, July 12, 2012

Session 13: Future Directions in 3D Materials Science
Room: Exhibit Hall

8:15 AM	**Invited**: **Exploiting Advances in Microscopy for Direct 3D Characterization of Materials**: *Hamish Fraser*[1]; Daniel Huber[1]; John Sosa[1]; Brian Welk[1]; Robert Williams[1]; Peter Collins[2]; [1]The Ohio State University; [2]University of North Texas
8:45 AM	**Invited**: **The Five Parameter Grain Boundary Character Distribution of a TWIP Steel Determined from Three-dimensional Data Sets**: Hossein Beladi[1]; *Gregory Rohrer*[2]; [1]Deakin University; [2]Carnegie Mellon University
9:15 AM	**Invited**: **A Workshop to Promote the Use of High-energy X-ray Diffraction Experiments and Detailed Computational Analyses for Understanding Multiscale Phenomena in Crystalline Materials**: *Matthew Miller*[1]; Robert Suter[2]; Ulrich Lienert[3]; Armand Beaudoin[4]; [1]Cornell University; [2]Carnegie Mellon University; [3]Argonne National Laboratory; [4]University of Illinois at Urbana Champaign
9:45 AM	**Break**
10:00 AM	**Invited**: **Future Directions for 3D Imaging in the (S)TEM**: *Paul Midgley*[1]; [1]University of Cambridge
10:30 AM	**Invited**: **3D Materials by Design: From Genome to Flight**: *Greg Olson*[1]; [1]Northwestern University
11:00 AM	**Invited**: **The Critical Role of Digital 3D Structure in Advanced Materials Research and Development**: *Julie Christodoulou*[1]; [1]Office of Naval Research
11:30 AM	**Panel Discussion**

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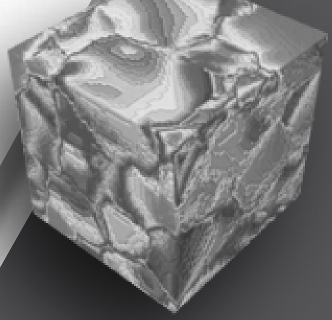

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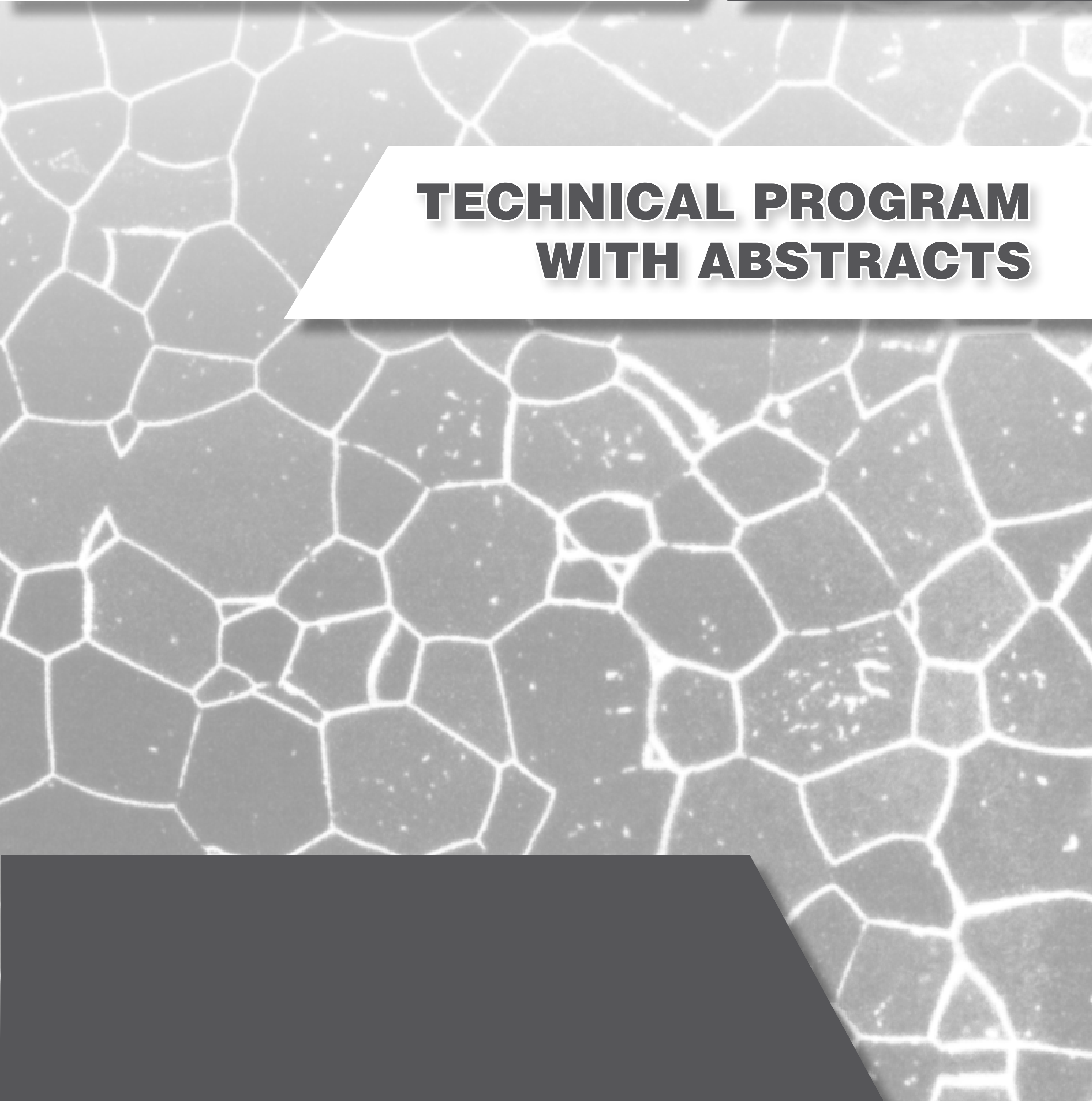

Plenary Session

Sunday PM July 8, 2012 | Room: Exhibit Hall | Location: Seven Springs Mountain Resort

7:30 PM Introductory Comments

7:35 PM Plenary
Perspectives on Materials Science in 3D: *Dorte Jensen*[1]; [1]DTU Risø

Materials characterization in 3D has opened a new era in materials science. Such characterization has already revealed that many conceptions and models developed based on 2D experimental characterizations do not give the full description of fundamental processes and may even be incorrect. Much work remains (i) using the new 3D techniques in combination with more traditional experimental tools (ii) developing new analyses and imaging tools to interpret the vast amounts of data typically recorded with the 3D techniques and (iii) obtaining new more complete and correct understanding of the underlying mechanics. In this talk, some of the original needs and visions behind developing one of the new 3D techniques, namely the three-dimensional x-ray diffraction (3DXRD) method, are presented. The present status of materials science in 3D is illustrated by examples. Finally challenges and suggestions for the future relating to hardware evolution, data analysis and materials science are discussed.

Applications of 3D Experimental Techniques Across Length Scales

Monday AM July 9, 2012 | Room: Exhibit Hall | Location: Seven Springs Mountain Resort

8:15 AM Invited
Development of Multi-modal 3D Characterization Systems to Quantify Grain & Precipitate Microstructural Features in Aerospace Alloys: *Michael Uchic*[1]; Michael Groeber[1]; Megna Shah[2]; Patrick Callahan[1]; Adam Shiveley[3]; Michael Chapman[3]; [1]Air Force Research Laboratory; [2]UES, Inc.; [3]SOCHE

In order to rapidly quantify key attributes of grain and precipitate ensembles in structural alloys, two different serial sectioning systems have been developed to examine material volumes ranging in scale from 50 \956m^3 to 1 cm^3. For smaller length scales, custom software scripts have been developed to control commercially-available FIB-SEMs outfitted with EDS and EBSD detectors. For material volumes > 0.001 mm, a novel 3D characterization instrument has been constructed that couples a SEM with EDS and EBSD detectors to a precise mechanical polishing system. Importantly, the collection of multi-modal data— crystallographic and spectral x-ray maps, as well as electron-optic images—greatly improves the ability of software codes to segment key microstructural features such as grains and second phases compared to conventional image-based segmentation. The talk will discuss the salient features of both serial sectioning systems, as well as present results from selected studies of Ni and Ti alloys.

8:45 AM Invited
Three-dimensional Characterization of Dislocation-Defect Interactions: *Ian Robertson*[1]; Josh Kacher[1]; [1]University of Illinois at Urbana-Champaign

Transmission electron microscopes have played a critical role in building our knowledge base of the atomic structure and composition as well as the electronic and magnetic state of materials. This information is a two-dimensional snapshot of the material state and requires a posteriori analysis to reveal the reaction or processing pathway, or to correlate with a macroscopic property. However, using electron tomography it is feasible to reconstruct from a series of images a three-dimensional view of the internal structure in an electron transparent foil. In this talk, I will demonstrate how electron tomography can be applied to dislocation/defect interactions using diffraction contrast imaging. Challenges to using diffraction contrast imaging, such as overcoming the invisibility criteria and introducing a three-dimensional coordinate system in the tomogram, will be presented and addressed. Unique insight available through three-dimensional characterization into dislocation interactions with grain boundaries, precipitates, and other dislocations will be given.

9:15 AM Invited
Acquisition of 3D Datasets for Property Prediction: *Tresa Pollock*[1]; McLean Echlin[1]; Alessandro Mottura[1]; Chris Torbet[1]; [1]University of California Santa Barbara

The development of high fidelity material property models often requires three-dimensional information on the distribution of phases, grains or extrinsic defects. Concurrently, information on orientation and spatial distribution of elements may also be essential. Acquisition of this information in appropriate representative volume elements ultimately limits the use of specific tomography techniques. The use of femtosecond lasers for rapid layer-by-layer ablation provides new capabilities in terms of the volume of material that can be sampled as well as new opportunities for multimodal analysis. The characteristics of datasets on Ni-base alloys and steel required for modeling of fatigue and fracture will be discussed. Femtosecond laser-based datasets will be presented for these materials and the use these datasets to predict properties will be discussed. Future opportunities for in-situ and ex-situ variants of the FSL technique will be discussed.

9:45 AM Invited
Connecting Atomic Scale Crystallography and Chemistry through Atom Probe Tomography: *Peter Felfer*[1]; Julie Cairney[1]; Vicente Araullo-Peters[1]; Saritha Simundrala[1]; [1]University of Sydney

In crystalline materials, the local chemistry at crystal defects such as grain boundaries, dislocations or second phases is intimately linked to their crystallographic nature and vice versa. In order to connect the two, both the knowledge of the crystal orientation of the crystallites adjacent to the defect and the distribution of the elements is required. In many cases,atom probe tomography (APT) can be used to obtain this information. Due to the nature of the field evaporation process, which is the basis of APT, information about the crystal orientation is often contained in the distribution of the field evaporated atoms and periodicities in the field evaporation sequence. In this talk, we present methods that allow for the mapping of crystal orientations in various metallic materials including steels, superalloys and nano-crystalline aluminium. We will introduce novel methods of quantifying the local chemistry around the feature, which can becorrelated with the crystallographic information.

10:15 AM Question and Answer Period

10:30 AM Break

Applications of 3D Experimental Techniques Across Length Scales: Destructive Techniques

Monday AM July 9, 2012 | Room: Exhibit Hall | Location: Seven Springs Mountain Resort

10:45 AM
3D Multi-scale Electron Microscopy for Nano-scale Carbide Mapping in a Tempered 9 Cr Martensitic Steel: *Niven Monsegue*[1]; Xin Jin[2]; Nana Kwame Yamoah[1]; Jeff Hawk[3]; William Reynolds[1]; Ge Wang[1]; Mitsuhiro Murayama[1]; [1]Virginia Tech; [2]Tsinghua University; [3]U.S. Department of Energy

This work highlights the benefits of a new transmission electron microscopy computed tomography enhanced reconstruction technique called Compressed Sensing (CS). Using CS, improvements in reconstruction accuracy over Simultaneous Iterative Reconstruction Technique and Back Projection algorithms was observed; 3D reconstruction was performed using fewer projections than traditionally required. Combining TEM-CT and SEM-Electron Back Scatter Diffraction, a comprehensive microstructure evolution analysis was performed on the steel alloy COST B2. COST B2 is a 9-12% Cr martensitic steel used in various Ultra Super Critical coal power plants; however, limited information exists on this alloy's microstructure transformation while under creep. In this study we compare the microstructures of COST B2 that has been creep tested and as-cast. Size, shape, and distribution of carbides within the alloy matrix, especially nano-scale carbide phases during creep test, were analyzed thus showing the structure-property relationship of carbides in COST B2 with respect to creep resistance.

11:05 AM

Combining Atom-probe Tomography with Focused-ion Beam Microscopy for Targeted 3D Materials Characterization with Sub-nanometer Resolution: *Dieter Isheim*[1]; David Seidman[1]; [1]Northwestern University

The 3D spatial analytical resolution ability of an atom-probe tomographic (APT) microscope combined with the capabilities of a dual-beam focused-ion beam (FIB) microscope for targeted specimen preparation is a powerful method for structural and chemical compositional characterization of materials at the subnanometer scale. Employing cutting, deposition, and manipulation techniques in the FIB it is possible to target specific microstructural features of almost any material. Laser-assisted APT yields a faithful 3D reconstruction with subnanometer spatial resolution and 10 atomic ppm analytical sensitivity. We discuss preparation methods and APT results for a variety of materials, such as catalytically grown silicon nanowires, pre-solar nanodiamond particles isolated from meteorites, oxide formation in crack walls and crack tips in stress-corrosion cracked nickel-base superalloys, martensite/austenite interfaces in high-strength steels, interface sharpness of multilayer structures in electronic materials, cluster and precipitate formation in PbTe-based thermoelectric materials, and dopant distributions in Mn-doped PbS nanowires.

11:25 AM

3D Orientation Imaging with Transmission Electron Microscopy: *Søren Schmidt*[1]; Haihua Liu[2]; Andy Godfrey[3]; Henning Poulsen[1]; Xiaoxu Huang[1]; [1]Risoe DTU, Technical University of Denmark; [2]California Institute of Technology; [3]Tsinghua University

We present a novel methodology for obtaining 3D orientation maps with spatial resolution of 1 nm in foils with few hundreds nm thickness. The method utilizes Transmission Electron Microscopy (TEM) in conical dark field scanning mode for data acquisition, where images are collected over a wide range of beam and sample tilts. The reconstruction algorithms are based on existing orientation imaging software for use with 3DXRD (Three dimensional X-ray Diffraction) microscopy. The methodology, algorithms and examples are presented along with potential applications.

11:45 AM Break

12:00 PM

Electron Tomography in Aberration-corrected Transmission Electron Microscopes: *Peter Ercius*[1]; [1]National Center for Electron Microscopy

Aberration-correction has pushed the limits of transmission electron microscopes (TEM) to sub-Angstrom resolution such that the atomic structure of materials is readily visible. Such high-resolution TEM images are being routinely used to analyze nano-structures with important applications in energy, catalysis, electronics and many more fields. However, these are only projections of complex three-dimensional structures, and the lost information is critical to determine the function of nano-structures. Techniques such as electron tomography and single-particle analysis have been routinely used in electron microscopy to recover the lost information along the projection direction from a series of images at many different viewing angles, but determining the exact positions of all atoms within a structure requires some new acquisition and processing techniques. I will discuss the imaging and tilting capabilities of a new generation of microscopes and different data acquisition/reconstruction techniques which should allow full atomic-scale three-dimensional reconstruction.

12:20 PM

FIB/SEM Determination of Sub-surface Damage Caused by Micro-tribology Scratching of WC/Co Hardmetal Samples: *Mark Gee*[1]; Ken Mingard[1]; Andrew Gant[1]; Helen Jones[1]; [1]National Physical Laboratory

WC/Co hardmetals are composite materials that are used in many wear resistant applications. Micro-tribology experiments were carried out on polished samples of WC/Co as model single point abrasion tests to determine the microstructural mechanisms of wear. The mechanisms of wear included plastic deformation and micro-fracture of the WC grains leading to fragmentation of the grains with re-embedment in the binder phase to form layers covering and protecting further damage to the surface. Ion beam milling with FIB / SEM sectioning and 3D reconstruction was used to characterise the sub-surface damage that occurred beneath scratches. It was found that specific WC grains at the surface fractured, with an increasing number of fragmented grains as the severity of the test parameters was increased. This led to an increased thickness of the re-embedded layer. The likelihood of fracture for specific grains was correlated with the orientation of the grains through EBSD analysis.

Applications of 3D Experimental Techniques Across Length Scales: Structure-Property Relationships

Monday AM — Room: Sunburst
July 9, 2012 — Location: Seven Springs Mountain Resort

10:45 AM

Atom-probe Tomography and the Science of a New Class of High-temperature Al-Sc Based Alloys: *David Seidman*[1]; David Dunand[1]; [1]Northwestern University

We have developed and studied from a fundamental scientific point-of-view novel Al-Sc-ME-TM-RE (ME = metal: Li, Mg, Si; TM = transition element: Ti, Y, Zr; RE = rare earth element: La and lanthanides) alloys, which exhibit excellent coarsening- and creep resistance at temperatures upwards of 673 K. We rely crucially on the use of atom-probe tomography (APT), which provides direct space three-dimensional information concerning microstructure and chemical compositions on a subnanometer scale. APT provides the necessary physical quantities to understand and model the high-temperature mechanical properties. Specifically, the following microstructural properties of precipitates are measured: (a) volume fraction; (b) mean radius; (c) number density; (d) size distributions in three-dimensions; and (d) chemical compositions of the matrix and precipitate phases as a function of aging temperature and time. This quantitative information is utilized, for example, in the Mohles code to understand the mechanism(s) of plastic deformation at ambient and elevated temperatures.

11:05 AM
3D Investigation of Cracking Behavior in a Ni Superalloy: *Andrew Deal*[1]; David Rowenhorst[2]; Brandon Laflen[1]; Ian Spinelli[1]; Anthony Barbuto[1]; Yuchi Huang[1]; Timothy Hanlon[1]; [1]GE Global Research; [2]Naval Research Laboratory

The high temperature fatigue performance of Ni-base superalloys is critical to gas turbine applications and as such, requires a more fundamental understanding when designing and producing turbine components. To investigate the relationship to local microstructure, a fatigue specimen was cycled under conditions designed specifically to result in intergranular propagation. Prior to failure, the test was interrupted and a 3D data set was reconstructed destructively from optical and EBSD slices taken from around the tip of the growing crack. The data set was investigated to understand the character of grain boundary planes along the crack front with respect those of the bulk material.

11:25 AM
Building Three Dimensional Microstructure of AA5754 Aluminum Sheet for Formability Simulation: *Jonathan Rossiter*[1]; Kaan Inal[1]; Raja Mishra[2]; [1]University of Waterloo; [2]General Motors R&D

This work represents the first application of building three-dimensional (3D) microstructure for numerical analysis that employs a Dual Beam Focused Ion Beam (FIB) in conjunction with Electron Backscatter Diffraction (EBSD) to obtain real grain and particle distribution data in AA5754 aluminum sheet. 3D serial sectioning of AA5754 samples were performed using a Zeiss N-vision Dual Beam FIB equipped with TSL EBSD detection. Individual sections were aligned and processed using in-house algorithms to create 3D finite element (FE) meshes containing grain and particle information. The FE meshes were then used in crystal plasticity theory based simulations for formability analysis to evaluate the role of particles as well as grain orientations and morphologies on strain localization. This paper provides a comparison between this approach and the 3D microstructure reconstruction approach from 2D EBSD data to highlight the indispensability of real microstructure information in identifying triaxiality hotspots leading to failure of Al alloys.

11:45 AM Break

12:00 PM
The TriBeam System: Femtosecond Laser Based Serial Sectioning: *McLean Echlin*[1]; Alessandro Mottura[1]; Tresa Pollock[1]; [1]UC Santa Barbara

In-situ material removal has been increased by 4-5 orders of magnitude over existing FIB techniques by incorporating a femtosecond laser into a microscope with both ion and electron beams. This tool has significant potential for a number of material removal applications, such as TEM sample preparation, laser induced breakdown spectroscopy (LIBS), and serial sectioning. The significant increase in the rate of material removal has permitted the milling of volumes that are up to 1mm^3. Serial sections have been collected with multi-mode detectors including EBSD, EDS mapping, and SEM images. The low imparted dislocation damage and surface roughness from femtosecond laser machining does not interfere with the collection of EBSD and EDS maps with a good confidence index. A reconstructed EBSD dataset of a polycrystalline nickel with grain size of 10-40 μm is presented with statistical analysis of the microstructure.

12:20 PM
Characterization and Modeling Via Three-dimensional Reconstructions of Laser Welds in Stainless Steel: *Jonathan Madison*[1]; [1]Sandia National Laboratories

Edge joints machined by continuous wave Nd:YAG laser in 304-L stainless steel, have been produced to yield assorted weld-pool widths, penetration depths, varying microstructures and differing porosity levels. Acquisition of three-dimensional reconstructions via micro-computed tomography and serial-sectioning have allowed for qualitative and quantitative characterization yielding both averages and distributions of key microstructural features. Challenges and milestones associated with using these reconstructions as direct inputs for mechanical response finite element models will also be highlighted and discussed. With respect to characterization, variability in shape, concentration and arrangement of voids, phases and grains are considered for short and long range order and their respective impact upon anticipated experimental variability and deformation. With regard to modeling, multiple deformation modes and rates are evaluated and insights into void linkage, coalescence and failure mechanisms are explored.

Poster Session 1: 3D Interfaces, Microstructural Evolution, Structure-Property Relationships

Monday PM	Room: Exhibit Hall
July 9, 2012	Location: Seven Springs Mountain Resort

P1-01: 3D Analysis of Surface Blisters, Subsurface Bubbles, and Underlying Microstructures of Implanted Metals: *John Smugeresky*[1]; Dan Huber[2]; Robert Kolasinski[1]; Don Cowgill[1]; John Sosa[2]; Hamish Fraser[2]; [1]Sandia National Laboratories, CA; [2]Ohio State University

Tungsten, nickel, and palladium are used in different applications that involve implantation of hydrogen or helium. Subsequent heating promotes diffusion which can lead to surface blister formation. For tungsten, used in the first wall of fusion reactors, it is of interest to determine if the radioactive species will stay trapped or be recycled back into the plasma. For nickel and palladium used for hydrogen storage or isotope separation applications, the radioactive decay of tritium into helium and its trapping within the solid acts as a tritium purification process. 3D analysis using FIB serial sectioning to locate where subsurface nanoscale bubbles form and FIB TEM foil extraction at those specific sites was used to test models for bubble formation. The underlying microstructure and void formation were characterized to determine its extent and to compare mechanisms of bubble formation leading to blistering. This paper compares the differences between the three metals.

P1-02: 3D Characterization of Recrystallization Boundaries: *Yubin Zhang*[1]; Dorte Juul Jensen[1]; [1]Danish-Chinese Center for Nanometals, Materials Research Division, Risø National Laboratory for Sustainable Energy, Technical University of Denmark

The migration of recrystallizing boundaries is a key process during recrystallization, and controls microstructural and textural evolution. Detailed two-dimensional (2D) investigations show that recrystallizing boundaries consist of many protrusions and retrusions on a local scale, and investigations of the formation mechanism of pro-/re-trusions are shown to be significant for understanding the migration of recrystallizing boundaries. In the present investigation, a 3D volume containing both a recrystallizing grain and deformed matrix separated by a recrystallizing boundary has been characterized using 3D electron backscattering pattern (3D-EBSP) techniques in a scanning electron microscope combined with focus iron beam. From the computer-reconstructed 3D-EBSP maps, some key information, such as the 3D shape of the recrystallizing boundary and the full 3D information of the deformed matrix in front of the recrystallizing boundary, has been obtained. These informations are important for the understanding of the formation of pro-/re-trusions and can only be obtained by 3D techniques.

P1-03: 3D Microstructural Architectures for Metal and Alloy Components Fabricated by 3D Printing/Additive Manufacturing Technologies: *E. Martinez*[1]; L. E. Murr[1]; K. Amato[1]; J. Hernandez[1]; P. Shindo[1]; S. Gaytan[1]; D. Ramirez[1]; F. Medina[2]; R. Wicker[2]; [1]University of Texas at El Paso, Metallurgical and Materials Engineering; [2]University of Texas at El Paso, W. M. Keck Center for 3D Innovation

The layer-by-layer building of monolithic, 3D metal components from selectively melted powder layers using laser or electron beams is a novel form of 3D printing or additive manufacturing. Microstructures created in these 3D products can involve novel, directional solidification structures which can include crystallographically oriented grains containing columnar arrays of precipitates characteristic of a microstructural architecture. These microstructural architectures are advantageously rendered in 3D image constructions involving light optical microscopy and scanning and transmission electron microscopy observations. Microstructural evolution can also be effectively examined through 3D image sequences which, along with x-ray diffraction (XRD) analysis in the x-y and x-z planes, can effectively characterize related crystallographic/texture variances. This paper compares 3D microstructural architectures in Co-base and Ni-base superalloys, columnar martensitic grain structures in 17-4 PH alloy, and columnar copper oxides and dislocation arrays in copper.

P1-04: 3D Microstructural Characterization of Uranium Oxide as a Surrogate Nuclear Fuel: Effect of Oxygen Stoichiometry on Grain Boundary Distributions: Karin Rudman[1]; Patricia Dickerson[2]; Darrin Byler[2]; Robert Dickerson[2]; Harn Lim[1]; Robert McDonald[1]; *Pedro Peralta*[1]; Kenneth McClellan[2]; [1]Arizona State University; [2]Los Alamos National Laboratory

The initial microstructure of an oxide fuel can play a key role in its performance. At low burnups, the diffusion of fission products can depend strongly on grain size and grain boundary (GB) characteristics, which in turn depend on processing conditions and oxygen stoichiometry. Serial sectioning techniques using Focused Ion Beam were developed to obtain Electron Backscatter Diffraction (EBSD) data for depleted UO2 pellets that were processed to obtain 3 different oxygen stoichiometries . The EBSD data were used to create 3D microstructure reconstructions and to gather statistical information on the grain and GB crystallography, with emphasis on identifying the character (twist, tilt, mixed) for GBs that meet the Coincident Site Lattice (CSL) criterion as well as GBs with the most common misorientation angles. Data on dihedral angles at triple points were also collected. The results were compared across different samples to understand effects of oxygen content on microstructure evolution.

P1-05: A Three-dimensional EBSD Investigation on the Distribution of Recrystallization Embryo in the Grain Boundary Regions of a Cold Rolled Low Carbon Steel: *Nasima Afrin*[1]; Md Zakaria Quadir[1]; Michael Ferry[1]; [1]University of New South Wales

A three dimensional (3D) electron backscatter diffraction (EBSD) investigation was conducted in the grain boundary regions of a micro-alloyed steel following moderately high rolling deformations. It has been found that there are two categories of deformation structures in steels. Among them the highly fragmented grains belong to a particular set of orientations, which are known as so called gamma fibre. The grains in this class are of particular interest because of being the early nucleation sites during recrystallization annealing. In this investigation a boundary region of two highly fragmented grains has been investigated to find the nature of orientation gradients in the adjacent areas. The 3D distributions of the deformation features are highlighted in respect to their surrounding materials and then an analogy is drawn to examine their capability to be the nucleation sites in the light of conventional recrystallization science.

P1-06: A Toolbox for Geometric Grain Boundary Characterization: *Krzysztof Glowinski*[1]; Adam Morawiec[1]; [1]Institute of Metallurgy and Materials Science, Polish Academy of Sciences

Properties of polycrystalline materials are affected by grain boundary networks. The most basic aspect of boundary analysis is the boundary geometry. We have been developing computer software for geometric boundary characterization based on five macroscopic boundary parameters. It is applicable to both individual boundaries in bicrystals and large boundary data sets. The purpose of the package is to allow for determination whether a boundary can be described as CSL, tilt, twist, symmetric, symmetric tilt etc. Since calculations on experimental, i.e., error affected data are assumed, the software also provides distances to the nearest geometrically characteristic boundaries. In the case of large boundary data sets, the goal is to allow for estimating the frequencies of occurrence of characteristic boundaries. The software will have a number of other functions helpful in grain boundary analysis including some visualization of boundary geometry and boundary structure. It allows for non-cubic crystal symmetries.

P1-07: An EBSD-based Characterization of Fe-9Ni and Fe-12Mn Martensitic Steels: *Christopher Kinney*[1]; Ken Pytlewski[1]; Y. Adachi[2]; J.W. Morris[1]; [1]University of California, Berkeley; [2]Kagoshima University

This paper presents an EBSD-based characterization of the microstructure of Fe-9Ni and Fe-12Mn martensitic steels, emphasizing its control of strength and toughness. The complex packet-block-lath structure of dislocated martensitic steel has been clarified in recent years as EBSD analyses have been applied. The laths are related to the parent austenite through the Kurdjumov-Sachs crystallographic relations, which define 24 crystallographically distinct variants. A packet contains the six of these that share a common {110} plane. A block contains the two of these six that share a common "Bain axis", and hence common {100} planes. For fundamental reasons, the blocks are the microstructural element that governs cleavage fracture, while, depending on the cleanliness of the boundaries, the strength may be controlled by either the block size or the prior austenite grain size. While Fe-9Ni and Fe-12Mn steels obey the same crystallographic rules, the two alloys have dramatically different microstructures and properties.

P1-08: Bainitic Microstructures in Weld Heat Affected Zones Studied by Electron Back-Scattering Diffraction: Joacim Hagström[1]; Bevis Hutchinson[1]; Oskar Karlsson[1]; Philip Withers[2]; *Ali Gholinia*[2]; [1]SwereaKIMAB AB; [2]The University of Manchester

Steels having microstructures consisting of bainite are growing rapidly in industrial importance. Their mechanical properties are of considerable interest and it is an important aim to be able to rationalise them on the basis of their microstructures. These structures are extremely complex and difficult to understand on the basis of normal 2D sections. They are also frequently very fine scale structures. The present work includes bainitic structures produced during simulated strip steel processing and also HAZ structures in different steels simulating the effect of welding with different heat inputs. These structures are associated with widely differing mechanical properties as will be explained. The 3D experiments have been preceded by extensive conventional EBSD studies on the same materials. The 3D-EBSD data are being used to gain new information about the bainitic microstructures in terms of: grain (lath) size and form, inter-penetration of laths, relationships between crystallography and shape, orientations and misorientations.

P1-09: Atomic Density Function 3D Modeling of Crystal Growth with Different Symmetry: *Helena Zapolsky*[1]; Armen Khachaturyan[1]; Renaud Patte[1]; [1]University of Rouen

Recently, atomic density function (ADF) model has been proposed to describe the realistic aspects of material dynamics, including grain growth, ductile fracture, epitaxial growth, solidification processes and reconstructive phase transitions at atomic scale. In spite of the ADF method has been successfully applied to describe qualitatively a wide range of phenomena, its predictive capability and quantitative description of phase transition remains largely unexplored. One of the main questions is how to evaluate the non-local party of the free energy of system. In our work, using ADF 3D simulations, we investigated the different interaction potentials and their influence on the lattice symmetry. In particularly, it was shown that a double well potential can stabilize the quadratic structure in 2D and 3D simulations.

P1-10: Computing Fatigue Properties of Polycrystalline Ni-based Superalloy Microstructures using an Image-based Computational Approach: *Bin Wen*[1]; Nicholas Zabaras[1]; [1]Materials Process Design and Control Laboratory

An efficient full-field method of computing the local and overall responses of elasto-viscoplastic polycrystalline microstructures based on fast Fourier transform (FFT) algorithm is presented. This formulation takes realistic microstructure images as the input and estimates their mechanical responses/properties under periodic boundary conditions without requiring complex finite element discretization. Effective stress-strain response, local mechanical fields and crystallographic texture of deformed polycrystalline microstructures are captured. Special interest is given to the fatigue indicator parameters (FIPs) of Ni-based superalloy IN100 to study its microstructure-sensitive fatigue properties. The results are compared with crystal plasticity finite element method (CPFEM) solutions. This image-based model is shown to have better performance for the same resolution.

P1-11: Effect of Grain Boundary Properties on Evolution of Lattice Orientations: *Jaehyung Cho*[1]; Chang-Seok Oh[1]; [1]Korea Institute of Materials Science

Grain boundaries can be defined by five parameters, plane normal (2-DOF) and misorientation angle/axis (3-DOF) between two adjacent grains. Several grain boundary properties, which are usually found in the deformed fcc metals, are designed and their effect on evolution of lattice orientation during uniaxial tension is discussed. Three-dimensional crystal plasticity finite element method (CPFEM) was introduced. Various combinations of grain boundaries were modeled. In order to characterize the features of microstructural evolution, orientation average and correlation parameters between misorientation and its special distribution are used. Inter- and intra-grain structures are also investigated using the spatial distribution of lattice orientation. It is evident that with deformation, more spreading of lattice orientations was found.

P1-12: Elastic Behavior of the Percolating Eutectic Structure of a High Pressure Die Cast Magnesium Alloy: *Bao Zhang*[1]; Anumalasetty Nagasekhar[1]; Carlos Caceres[1]; [1]The University of Queensland

The 3D configuration of the ($Mg_{17}Al_{12}$) β phase intermetallic microstructure in the AZ91D alloy obtained using dual beam FIB tomography was incorporated into an FEM code and loaded in tension. The structure stiffness is consistent with bending-dominated behavior.

P1-13: Fragmentation of a Steel Ring under Explosive Loading: *Jeremy Schreiber*[1]; Ivi Smid[1]; Timothy Eden[1]; [1]Penn State

There is a great deal of interest in the behavior of metallic materials under high strain rate loading. Finite element analysis can be used to model these materials with a reduction in the amount of experimentation needed for characterization. In a novel approach, a finite element model of a metallic ring under high strain rate loading was developed using the Johnson-Cook failure model in Abaqus. The ring was modeled both axisymmetrically and in 3-D to help ensure accuracy in results. Failure was assumed to occur when the failure strain was exceeded, causing element deletion. Based on this approach, and comparing with experimental data, a failure strain of 1x10^-5 is predicted. Results of both axisymmetric and 3-D were found to be within 3% of each other with respect to maximum stresses, and failure modes were identical. The effects of material changes and different loading conditions on microstructure and fragmentation are compared.

P1-14: Gas Fast Reactors Fuel Claddings: Braids Densification Simulations and Equivalent Thermal Conductivities Calculations: *Sylvain Chupin*[1]; Patrick David[1]; Denis Rochais[1]; Francois Guillet[1]; Laurent Chaffron[2]; [1]CEA-Le Ripault; [2]CEA-Saclay

The conception and realisation of fuel claddings for use in fast neutron spectrum constitutes a very high challenge for material science. Claddings must ensure, at high temperature, under high dose conditions, the functions of mechanical structuration of fission product containment, and heat removal. To help resolving this challenge, composite ceramics naturally appears interesting. SiC braidings with CVI SiC deposit are then studied. From the process and the final shape of such made composites, two tools have been developped to numerically create reallistic microstructures of fuel claddings. The first one is able to create braid microstructures depending on the number of threads, shape of threads, angle of braiding, etc. The second one has been developped to simulate the CVI densification of the previously created weaves. Thermal calculations on various of these numeric microstructures are done to estimate the evolution of homogeneous equivalent longitudinal and tranverse thermal conductivities for different claddings microstructures.

P1-15: Gating System Optimisation Design Study of a Cast Automobile Component Made in Aluminium Alloy: *Eyitayo Olakanmi*[1]; [1]Federal University of Technology

This study aims to improve the structural integrity of a cast automobile component made in an aluminium alloy by employing Pro-Engineer software to simulate the mould filling and the casting solidification for achieving accurate casting design and proper design of gating system. Different designs of the gating and risering systems for the cast automobile component were explored. Gating system parameters such as ingate height, ingate width, runner height, runner width, and position of the gating system were optimised by Taguchi design of experiment with consideration of performance characteristics of the automobile component (filling velocity, micro porosity, residual stress, and tensile strength). An orthogonal array, the signal to-noise (S/N) ratio, and analysis of variance (ANOVA) were used to analyse the effect of various gating designs parameters on the performance characteristics of the automobile component. Finally, specimens obtained from the different parts of the casting produced by optimised parameters were subjected to both microstructural and mechanical testing with a view to estimating the fraction/size of the porosity and the mechanical properties of the automobile component. The simulation results were then compared with the experimental findings, and then discussed. This study emphasises the rationale that casting designers and foundry men need to gain mutual understanding of each other's roles and challenges in order to employ computer software to optimise the design parameters for minimising rejects of cast automobile components in the foundry.

P1-16: Grain Boundary Networks in Polycrystalline Materials: Understanding Structure/Property Relationships: *Alexis Lewis*[1]; Andrew Geltmacher[1]; Siddiq Qidwai[1]; [1]Naval Research Laboratory

In this work, the microstructure of an austenitic stainless steel was reconstructed in three dimensions to characterize the 3D networks of grain boundaries, including both general high-angle boundaries and special coincident site lattice (CSL) boundaries. The microstructure is characterized using serial sectioning and EBSD, and the connectivity of the grain boundary networks is measured, for both an as-received specimen, and one which has been subjected to Grain Boundary Engineering (GBE) to increase the population of special CSL boundaries. Simulations of material response, particularly with respect to stress corrosion cracking and diffusional creep, were performed to predict the influence of special boundary network connectivity on material properties.

P1-17: In-situ Investigation of Damage and Strain Mechanisms in Structural Sheet Material via Synchrotron Radiation Laminography: Thilo Morgeneyer[1]; Lukas Helfen[2]; Francois Hild[3]; *Henry Proudhon*[1]; Ian Sinclair[4]; [1]Mines Paristech; [2]KIT; [3]ENS Cachan; [4]University of Southampton

In this study the opportunities that arise from synchrotron radiation laminography for 3D in-situ assessment of damage mechanisms in structural sheet material are shown. The technique is similar to tomography but allows to image objects that are extended in 2 dimensions. The initiation and propagation of cracks in two different aluminium alloys are investigated and different mechanisms are seen involving void growth, shear coalescence and also intergranular failure. The influence of stress state on fracture mechanisms can clearly be identified using samples that have sizes of several centimetres in the sheet plane. A first attempt to quantify damage evolution is made. In addition, a study is shown that tries to identify displacement fields and strain fields in 3D via digital volume correlation using the natural contrast of the material as markers.

P1-18: CANCELLED: K-phase in Fe-Al-Mn-C Alloys: Morphologies and Crystallographic Aspects: *Ian Zuazo*[1]; Helio Goldenstein[2]; Yves Bréchet[3]; Cyril Cayron[4]; [1]ArcelorMittal; [2]University of São Paulo; [3]SIMAP - Grenoble INP; [4]CEA-Grenoble, DRT/LITEN/DEHT/LCPEM

In duplex lightweight Fe-Al-Mn-C alloys the K-phase, $(Fe,Mn)_3AlC_x$, with a perovskite-type structure, precipitates at the austenite/ferrite interphase boundaries during both continuous cooling and isothermal heat treatments. A 3D metallographic investigation, using a deep etching technique, reveals the variety of true shapes and interconnections between fragmented morphologies occurring as a result of both types of treatments. EBSD investigations of these areas show the influence of the crystallographic features on the morphology selection revealing for instance that the K-phase needles prefer to growth with a Kurdjumov-Sachs orientation relationship with regard to the ferrite matrix. The combination of these two characterization techniques proved to be a powerful approach in this study.

P1-19: Microstructural Analysis of MgB_2 Superconducting Wires by Electron Microscopy and X-ray Computed Tomography: Satoshi Hata[1]; *Yusuke Shimada*[1]; Masatoshi Mitsuhara[1]; Ken-ichi Ikeda[1]; Hideharu Nakashima[1]; Akiyoshi Matsumoto[2]; Kazumasa Togano[2]; Hiroaki Kumakura[2]; Hitoshi Kitaguchi[2]; Jung Ho Kim[3]; Shi Xue Dou[3]; Jeff Gelb[4]; Wenbing Yun[4]; [1]Kyushu University; [2]National Institute for Materials Science; [3]University of Wollongong; [4]Xradia Inc.

The MgB_2 superconductor is promising from the viewpoint of future applications at a liquid hydrogen temperature. At present, the critical current density of MgB_2 wires is still lower than that of MgB_2 films with well-controlled microstructure. This is due to microstructural imperfectness: the existence of defects such as impurity phases, pores, cracks, etc. Here, we report the effectiveness of electron microscopy and x-ray computed tomography (CT) observations to study microstructure in MgB_2 superconducting wires fabricated by in-situ processes. Electron microscopy observation characterizes fine structures of these defects. On the other hand, x-ray CT observation reveals three-dimensional morphology and quantitative features of these defects. Combination of both the microscopy observations explains differences in critical current properties which depend on dopants and heat treatment conditions.

P1-20: Microstructure Visualization and Thermal Response Analysis of IF and Peritectic Mold Slag: *Pabitra Palai*[1]; Shainu Suresh[1]; T. K. Roy[1]; V. V. Mahashabde[1]; [1]Tata Steel Ltd., Jamshedpur, India

The microstructure and thermal response of mold slag used in continuous casting of interstitial free(IF) and peritectic steel were investigated. The network of cuspidine phase in Cao-SiO2-Al2O3 slag controls lubrication and heat transfer from solidifying steel. The cuspidine in crystallized slag forms 3-dimensional dendritic structure in the glass matrix. The evolution of chemistry and morphology of cuspidine phase were investigated using SEM, EDAX & EBSD. The results were used to study the heatflux and %Temperature Variation Coefficient(TVC). The cuspidine in IF slag composed of 27wt%Ca,20wt%Si whereas it is about 36wt%Ca and 15wt%Si in Peritectic slag. Low heatflux in peritectic slags over the IF is due to the higher CaO/SiO2 ratio, volume fraction and texture and is a specific characteristic of the slag for its excellent casting properties. Furthermore, the IF slag with reduced ratio of CaO/SiO2 ratio possesses a high heatflux capacity to achieve higher casting throughput.

P1-21: Numerical Analysis and Experimental Study on Dry Friction and Wear Performance of SiC 3D Continuous Network Ceramic Reinforced Fe-40Cr Alloy: *Yu Liang*[1]; Jiang Yanli[1]; Senkai Lu[1]; Ru Hongqiang[1]; Ming Fang[1]; [1]Key Laboratory of New Processing Technology for Nonferrous Metals & Materials, Ministry of Education, College of Materials Science and Engineering

The dry friction and wear behaviour of co–continuous composites SiC/Cu against SiC/Fe–40Cr was investigated with a ring on ring system. The wear tests were carried out under an applied load from 1.0 MPa to 2.5 MPa and sliding speed from 70 m/s to 105 m/s. The experimental result revealed that the main wear mechanisms for SiC/Fe–40Cr composites were two body abrasive wear and oxidative wear. Topographic examination of the worn surfaces revealed that the SiC/Fe–40Cr composite two-body abrasion predominated over its three-body abrasion in determining the friction and wear. The continuous network SiC ceramic as the reinforcement could avoid composite from the third body abrasive wear. The three-dimensional finite element method (FEM) analysis was used in this investigation. The wear and stress–strain behavior of the SiC/Fe–40Cr composite was calculated with an elastic-linear strengthen plastic deformation model by commercial software Solidwork Simulation. The present simulation showed good agreement with the experimental data.

P1-22: Numerical Implementations of Crystal Plasticity in the Spectral Representation: *Bogdan Mihaila*[1]; Marko Knezevic[1]; Andres Cardenas[2]; [1]Los Alamos National Laboratory; [2]New York University

We present several efficient numerical implementations of crystal plasticity in the spectral representation, with emphasize on high-performance aspects of the simulation. For illustrative purposes we apply this approach to a Taylor-type model for fcc poly-crystalline materials, and show that the spectral representation of crystal-plasticity is ideal for parallel implementations aimed at next-generation large-scale simulations of material deformation in the viscoplastic crystal-plasticity framework. Speedups of the simulation by three orders of magnitude relative to the conventional model are being reported.

P1-23: Calculation of Lorentz Force Field of the Innovation Cathode Cell: *Jiang Yanli*[1]; Yu Liang[1]; Feng Naixiang[2]; [1]Key Laboratory of New Processing Technology for Nonferrous Metals & Materials, Ministry of Education, College of Materials Science and Engineering; [2]School of Materials and Metallurgy, Northeastern University

The mathematical models of Lorentz force field of the conventional cell and innovation cathode cell were established in the paper. The result revealed that the Lorentz force distribution of the conventional cell and innovation cathode cell was different, but the value of Lorentz force was similar, the Lorentz force in aluminum liquid in the conventional cell became higher near the surface of the cathode, while it in aluminum liquid in the innovation cathode cell decreased at first, then increased at the concave of cathode, the Lorentz force in electrolyte of the conventional cell became higher away from the surface of the cathode, while it in electrolyte under the anode bottom of the innovation cathode cell was evenly distributed, then decreased in gap of the anode.

P1-24: Numerical Simulations of Compression Properties of SiC/Fe-20Cr Co-continuous Composites: *Yu Liang*[1]; Jiang Yanli[1]; Lu Senkai[1]; Ru Hongqiang[1]; Fang Ming[1]; [1]Key Laboratory of New Processing Technology for Nonferrous Metals & Materials, Ministry of Education, College of Materials Science and Engineering

The uniaxial deformation properties of a SiC/Fe–20Cr composite where both phases are continuous have been studied using the Solidwork simulation software applied the finite element method (FEM). The simulated results have shown that the composites are relatively anisotropy. Fe–20Cr matrix and SiC network ceramic exhibit different mechanical behaviour. The ultimate stress is found near the interface of composites. The configuration of SiC has relatively great influence on intensity and distribution of stress in the composite. The material behaves in a nearly bilinear manner defined by the Young's modulus and an elastic-plastic modulus. The large deformation appears inside Fe–20Cr matrix. The elastic deformation in the ceramic is accommodated by plastic deformation in the metal phase. Fe–20Cr and SiC can restrict each other to prevent from producing the strain under the load.

P1-26: Parallel Potts Model for Recrystallization and Sintering: Sukbin Lee[1]; *Anthony Rollett*[1]; [1]Carnegie Mellon University

A parallel code is described that implements a Potts Model in three dimensions with the capability to model late-stage sintering and Smith-Zener pinning of grain growth. The objective is to facilitate the development of materials processing that involves sintering and grain growth steps. The code is adapted from an existing parallel Potts model code that originated at Sandia [Miodownik et al. (2000) Scripta mater. 42 1173] Modifications will be described that accommodate crystallographic texture, recrystallization and pores. Examples of simulations are given to show how grain growth interacts with the pore content. A further extension is described for simulating recrystallization where the nucleation of new grains is controlled by externally supplied information (from measurement or simulation) on the spread in orientation at any given point. Since orientation spread increases monotonically with strain this form of the model provides a strain dependence of the recrystallized grain size.

P1-27: State-of-the-art in Finite Element Modeling of Microstructural Descriptors: *Veera Sundararaghavan*[1]; Shang Sun[1]; Abhishek Kumar[1]; [1]University of Michigan

Finite element (FE) models of microstructures are not of practical use in multiscale simulations due to their large computational cost. An alternate class of methods has been developed in recent years that describe microstructure evolution using descriptors rather than the actual microstructure itself. State–of–the–art models for evolving various orientation and stereological descriptors of a polycrystalline microstructure will be explained in this talk. In particular, we consider approaches to evolve the orientation distribution function (ODF), conditional orientation correlation function (COCF) and the grain size orientation distribution function (GSODF) during deformation processes. In our approach, the descriptors are represented using interconnected layers of finite element meshes. As the microstructure evolves, the reoriented neighborhood and strains close to a crystal are captured by updating probability fields in these finite element meshes. The texturing and strains predicted by the approach will be compared directly to FE deformation analysis to showcase its efficiency.

P1-28: Stress Relaxation in Polycrystals - Insights from Full-field Crystal Plasticity Fast Fourier Transform Approach: *Anand Kanjarla*[1]; Laurent Delannay[2]; Ricardo Lebensohn[1]; Huamiao Wang[3]; Carlos Tomé[1]; [1]Los Alamos National Laboratory; [2]Université Catholique de Louvain, Belgium; [3]McMaster University

In-situ study of materials by high energy X-ray and neutron diffraction techniques often involve maintaining the specimen at constant stress or constant strain while the required data is collected. Under these conditions, the local stress and strain fields are altered resulting in either stress relaxation under constant strain, or creep under constant stress conditions. It is vital to understand these phenomena in detail to correctly interpret the collected experimental data such as volume averaged internal lattice strains or spatial resolved mechanical fields. In this work, we model stress relaxation conditions in 3-D polycrystals using a recently developed elasto-viscoplastic Fast Fourier Transform approach. We report on the influence of crystallographic orientations, local neighborhood effects and grain boundary proximity on the local re-distribution of stresses under relaxation conditions. We compare our results to those obtained with a mean field elasto-viscoplastic model, to assess the role that stress localizations near grain boundaries play in the overall relaxation process.

P1-29: An Understanding of Embrittlement in Structural Materials Using 3D/4D Characterisation Methods: *Chiradeep Gupta*[1]; Hiroyuki Toda[1]; Masakazu Kobayashi[1]; Christian Schlacher[2]; Christof Sommitsch[2]; Peter Mayr[3]; Yoshio Suzuki[4]; Kentaro Useugi[4]; Akihisa Takeuchi[4]; [1]Toyohashi University of Technology; [2]Graz University of Technology; [3]Chemnitz University of Technology; [4]Japan Synchrotron Radiation Research Institute

The germane application of the state-of-the-art technique of micro-tomography is within the meso-length scales for understanding of failure phenomena in materials. However, only chronological mapping of the proliferation of voids or cracks by micro-CT may not be adequate for this purpose. Rather an investigation of spatial interaction of grain boundaries and particles during damage evolution would help to understand the mechanisms of embrittlement commonly observed in structural materials. In this presentation the power of the micro tomography technique available at the largest synchrotron source in world (SPring-8) is shown through investigations on hydrogen embrittlement in high strength aluminium alloys. Further a new paradigm concept is presented, in which the destructive technique of serial sectioning is combined with micro-CT images obtained non-destructively. The results of this new technique to yield unprecedented information on the mechanisms of failure by creep in 9-12% tempered martensitic steels are also shown.

P1-30: A Microscale Tension Test and Subsequent Serial Sectioning of an a+ß Titanium Alloy, Ti-6Al-2Sn-4Zr-6Mo: *Christopher Szczepanski*[1]; S.K. Jha[2]; R. Wheeler[3]; P.A. Shade[1]; J.M. Larsen[1]; [1]US Air Force Research Laboratory; [2]Universal Technology Corporation; [3]UES, Inc.

The properties of Ti-6Al-2Sn-4Zr-6Mo with a duplex microstructure have been extensively characterized via laboratory scale fatigue experiments. Via fractography and manual sectioning, material just beneath the fracture surface has been exposed and characterized with EBSD techniques. From these analyses, specific combinations of grain orientations have been identified as being susceptible to easy fatigue crack formation. However, in many cases, the fatigue crack initiation sites have a very similar appearance regardless of specimen lifetime. Thus, a microscale fatigue testing technique has been developed to monitor the activation of slip events and observe slip transfer to adjacent grains with in-situ techniques. A FIB-based serial sectioning experiment has been completed to section through a microspecimen following deformation. Characterization and analysis of this specimen volume will be presented to relate the observed slip events to specific grain orientations and neighborhoods.

P1-31: Multi-scale Tomographic Analysis of Ductile Fracture in Ultrahigh Strength Steels: *Stephanie Chan*[1]; Dave Rowenhorst[2]; George Spanos[3]; Erik Lauridsen[4]; Wolfgang Ludwig[5]; Greg Olson[6]; [1]NextGen Aeronautics, Inc. ; [2]Naval Research Laboratory; [3]Currently The Minerals, Metals, and Materials Society; [4]Risø National Laboratory; [5]Laboratoire MATEIS; [6]Northwestern University

Three-dimensional tomographic characterization and analysis tools have been developed to address microstructural evolution governing toughness, shear instability resistance, and fatigue strength in high-performance steels for naval applications. On the sub-micron scale, serial sectioning by focused ion beam (FIB) milling and scanning electron microscopy (SEM) resolved secondary grain-refining dispersions, microvoids, and primary particles in a modified-4330 steel shear band. On the micron scale, crack tips in modified-4330 and BlastAlloy160 steels were serial sectioned by metallographic polishing and optical microscopy to offer a three-dimensional picture of the void nucleation, growth, and coalescence stages of ductile fracture. Quantitative comparisons of the process zone, crack extension, zig-zag wavelength, crack opening displacement, void number density, void growth ratios, critical strain, and inclusion statistics illustrate the superior toughness of BlastAlloy160 over modified-4330 steel. Synchrotron X-ray computed microtomography of BlastAlloy160 crack tips validated serial sectioning methods by showing good corroboration in metrics of damage.

Image Processing of 2D and 3D Microstructural Data

Monday PM | Room: Exhibit Hall
July 9, 2012 | Location: Seven Springs Mountain Resort

6:30 PM Invited

Shape Analysis and Classification of Objects: *Brent Neal*[1]; John Russ[2]; [1]Milliken & Company; [2]North Carolina State University

Quantification of shape remains an area of active study in the field of image analysis and machine vision. We present a comparative survey of three approaches to shape measurement: classical dimensionless ratios, harmonic analysis, and invariant moments, showing their suitability for classification of objects and other statistical analyses, including quantitative structure-property relationships. We show that for topologically simple shapes and well controlled imaging conditions, all three methods can provide robust classification of objects.

7:00 PM Invited

Graph Cut Approaches for Materials Segmentation Preserving Shape, Appearance, and Topology: Jarrell Waggoner[1]; Jeff Simmons[2]; Marc De Graef[3]; *Song Wang*[1]; [1]University of South Carolina; [2]Materials and Manufacturing Directorate, Air Force Research Labs; [3]Carnegie Mellon University

Segmenting material images into underlying objects is an important but challenging problem given object complexity and image noise. Consistency of shape, appearance, and topology among the underlying objects are critical properties of materials images and can be considered as criteria to improve segmentation. For example, some materials may have objects with a specific shape or appearance in each serial section slice, which only changes minimally from slice to slice; and some materials may exhibit specific inter-object topology which constrains their neighboring relations. In this paper, we develop new graph-cut based approaches for materials science image segmentation. Specifically, these approaches segment image volumes by repeatedly propagating a 2D segmentation from one slice to another. We introduce different terms into the graph-cut cost function to enforce desirable shape, appearance, and topology consistency. We justify theeffectiveness of the proposed approaches by using them to segment sequences of serial-section images of different materials.

7:30 PM Question and Answer Period

7:45 PM

Simulation of FIB-SEM Images for Segmentation of Porous Microstructures: *Torben Prill*[1]; Katja Schladitz[1]; Christian Wieser[2]; [1]Fraunhofer ITWM; [2]Adam Opel AG

FIB tomography yields high quality 3D images of the microstructure of porous media combining serial sectioning using a focused ion beam with scanning electron microscopy (SEM). However, SEM images represent the projection of a slice of unknown thickness. In FIB tomography this leads to shine-through-artefacts preventing automatic segmentation of the 3D structure. To overcome these difficulties, we simulate the SEM process using a Monte-Carlo technique yielding accurate results, but being too slow for FIB-SEM requiring hundreds of SEM images for one dataset. Nevertheless, a quasi analytic description of the specimen and acceleration techniques cut down the computing time by orders of magnitude, allowing the simulation of FIB-SEM data. Simulated FIB-SEM image data at hand, we can use advanced image processing techniques like image features and machine learning to segment the 3D microstructure of highly porous media from the FIB-SEM data. This enables quantitative analysis and numerical simulations of macroscopic properties.

8:05 PM

A New Filtering Strategy for Noise Reduction on High Noise 3D Data Sets: *Steven Van Boxel*[1]; Nghia Vo[2]; Peter Lee[1]; Philip Withers[1]; [1]University of Manchester; [2]Singapore Synchrotron Light Source

Data sets of region of interest tomography scans inherently have high levels of moderately structured noise present. Common filtering approaches however often come at the cost of signal degradation, lowering the effective resolution. Advanced filters like e.g. the Perona-Malik filter perform much better, but are computationally costly. A new filtering strategy is presented that aims at achieving effective filtering already after a single iteration. This approach uses the Wiener and the Kuwahara filter. The Wiener filter is very effective in removing noise in regions away from phase boundaries, while the Kuwahara filter is designed to remove noise and sharpen boundaries at the same time. The effectiveness of the filtering approach is demonstrated on phantom data for different levels of noise and noise anisotropy. The usefulness of the filter approach is illustrated on region of interest tomography scans of lime stone and thermal barrier coatings.

8:25 PM Break

8:45 PM

Microstructural Characterization of Porous Shape Memory Alloys using X-ray Tomography: *David Rowenhorst*[1]; Catherine Tupper[2]; David Dunand[2]; [1]Naval Research Lab; [2]Northwestern University

There is increasing interests in the use of microstructured porous metallic systems, especially the in the use of shape memory alloys (SMA) due to their super elastic behavior making them ideal for use in biological implants and temperature activated actuators. In this presentation we will present methods for the characterization of structured porous alloys using desktop x-ray tomography. The large size and high density of these samples gives rise to a low signal to noise within typical desktop x-ray tomography systems, introducing unique image processing problems when segmenting the structure, a necessary step for linking the microstructure to performance. We will also discuss possible qualification metrics for systems of continuous networks.

9:05 PM

Model Based HAADF STEM Tomography: *Singanallur Venkatakrishnan*[1]; Lawrence Drummy[2]; Michael Jackson[3]; Marc Graef[4]; Charles Bouman[1]; Jeff Simmons[2]; [1]Purdue University; [2]AFRL; [3]BlueQuartz Software; [4]Carnegie Mellon University

There has been a growing interest in using High Angle Annular Dark Field (HAADF) signal from a STEM for tomography because it suppresses the dynamical scattering effects seen in bright field images of crystalline materials and produces an intensity approximately proportional to Z^2 in the region being imaged. Most efforts to reconstruct the object use the weighted back projection or SIRT algorithm which result in significant artifacts, especially in the limited angle regime of STEM tomography. Based on recent advances in X-ray tomography which have shown large improvements in the quality of reconstructions, we develop a model-based reconstruction algorithm for HAADF-STEM tomography. The method takes into account the process of image formation, the noise characteristics of the measurement and the inherent smoothness in the object to perform the reconstruction. Results from reconstruction on a data set of polystyrene functionalized TiO_2 nanoparticle assemblies will be presented.

9:25 PM
Energy-based Segmentation Methods for Micrograph Analysis: *Gunay Dogan*[1]; Stephen Langer[2]; Andrew Reid[2]; [1]Theiss Research; [2]National Institute of Standards and Technology

A fundamental step in image-based analysis of material microstructures is image segmentation, the task of extracting structures, such as the interfaces and the grains, from a micrograph. In this presentation, we describe effective segmentation methods that we have implemented, based on appropriately defined interface energies. The energies are defined such that they are minimized by given (guessed) interfaces or region boundaries if the interfaces align with apparent interfaces or edges in the image. To compute the minima of such energies, we propose efficient minimization algorithms that work in two stages: 1) topology optimization, which is fast and gives a good pre-segmentation, which can be also be used as the starting point for the second stage, 2) shape optimization, which iteratively aligns guessed interfaces with the actual interfaces in the image. Well-chosen gradient descent directions enable us to reduce the number of iterations needed, whereas taking an explicit Lagrangian approach and using adaptive discretizations reduce the computational cost per iteration while maintaining the accuracy. We intend to make the segmentation code available with OOF, a scientific computing platform developed at NIST for material microstructure analysis using the finite element method.

9:45 PM
Generalized Forward Projectors for the Iterative Reconstruction of Electron Beam Serial Sectioning Data Sets: *Marc De Graef*[1]; [1]Carnegie Mellon University

Conversion of serial sectioning data sets resulting from focused ion beam experiments into accurate 3D microstructure representations is often hindered by the fact that the electron images originate not just from the sample surface, but also from a sub-surface region. This sub-surface region is often of a size similar to that of the microstructural features that one is trying to reconstruct, which typically leads to segmentation problems. For instance, in Ni-based superalloys with a high γ volume fraction, the precipitates often appear to be connected in the reconstructions, but no such connections are apparent in visual inspections of the original SEM images. We will present a forward modeling approach to the automated iterative segmentation of such data sets; our approach takes into account the physics of the electron beam - sample interactions and facilitates the direct 3D segmentation of the microstructure. We will illustrate the approach using superalloy microstructure data.

Microstructure-Property Relationships in 3D

Tuesday AM	Room: Exhibit Hall
July 10, 2012	Location: Seven Springs Mountain Resort

8:15 AM Invited
4D Materials Science: In-situ X-ray Synchrotron Tomography of Deformation in Metallic Materials: *Nikhilesh Chawla*[1]; [1]Arizona State University

Advances in experimental methods, analytical techniques, and computational approaches, have enabled the development of three dimensional (3D) analyses. The study of 3D microstructures under an external stimulus (e.g., stress, temperature, environment) as a function of time (4D) is particularly exciting. X-ray synchrotron tomography provides a wonderful means of characterization damage in materials non-destructively. In this talk, I will describe experiments and simulations that address the critical link between microstructure and deformation behavior, by using a three-dimensional (3D) virtual microstructure obtained by x-ray synchrotron tomography. The approach involves capturing the microstructure by in situ deformation in an x-ray synchrotron, followed by x-ray tomography and image analysis, and 3D reconstruction of the microstructure. Quantitative analysis and incorporation of the microstructure into a powerful finite element modeling code for simulation can also be conducted. Case studies on fundamental deformation phenomena in metal matrix composites and Sn-based alloys will be presented and discussed.

8:45 AM Invited
Combining X-ray Microtomography with Full Field Finite Elements Method to Study 3D Cracking in Stuctural Materials: *Henry Proudhon*[1]; Jia Li[1]; Vincent Chiaruttini[2]; Thilo Morgeneyer[1]; Lucien Laiarinandrasana[1]; Samuel Forest[1]; Jean-Yves Buffière[3]; Wolfgang Ludwig[3]; [1]MINES ParisTech; [2]ONERA; [3]Université de Lyon

The increasing popularity and capability of X-ray tomography to image cracks and damage in three dimensions in a non destructive fashion brings forward a new way to validate large scale material failure simulations. A wide range of crack propagation case studies will be presented, ranging from cracks in notched polymer specimens and structural aluminum alloys to short crack propagation in a titanium alloy polycrystal. The incredibly rich knowledge brought at the micron scale by in situ imaging using either absorption, phase or diffraction contrasts, while the crack progresses, can often serve as direct input for full field simulations. Cracking mechanisms, direction and growth rate can therefore be tested and modeled at the appropriate scale (crazing in polymer materials, crystal plasticity in individual grains or linear elastic fracture mechanics for larger cracks). Automated image processing, meshing strategy and high performance computing will also be discussed.

9:15 AM Question and Answer Period

9:30 AM Break

Microstructure-Property Relationships in 3D: Fatigue, Failure and Deformation

Tuesday AM	Room: Exhibit Hall
July 10, 2012	Location: Seven Springs Mountain Resort

9:45 AM
3D Characterization and Modeling of Fatigue Cracks: *Anthony Rollett*[1]; Clayton Stein[1]; Reeju Pokharel[1]; Jonathan Lind[1]; Joseph Tucker[1]; Albert Cerrone[1]; Anthony Ingraffea[1]; Robert Suter[1]; Peter Kenesei[2]; Ulrich Lienert[2]; [1]Carnegie Mellon University; [2]Advanced Photon Source (APS)

Short fatigue cracks in nickel-based superalloys have been characterized in 3D using High Energy Diffraction Microscopy (HEDM), EBSD, and computed tomography (CT) to map out the crack positions within their embedding grain structure. The HEDM and CT are performed with high energy x-rays at the Advanced Photon Source (APS). The 3D orientation maps are used as input to computations of the full field stress-strain response. The likely origins of fatigue crack initiation in this material are discussed.

10:05 AM
3D Characterization and Modeling of the Influence of Porosity on Fatigue Properties of a Cast Al Alloy: *Jean-Yves Buffiere*[1]; Eric Maire[2]; Nicolas Vanderesse[3]; [1]Universite de Lyon INSA LYON ; [2]Universite de Lyon INSA LYON; [3]Ecole de Technologie Supérieure

In this work, three dimensional (3D) images of pores present in fatigue samples of a cast Al alloy have been obtained using laboratory X ray tomography. The 3D images have been used to generate realistic 3D Finite Element (FE) meshes of the samples microstructure at the pore level. A methodology for generating refined meshes has been developed. A new approach based on the conversion of FE data into 3D images is proposed and proves to be a fast, easy and reliable method for post-processing the results with the classical powerful techniques of 3D image analysis. Correlations between the fatigue lives of the investigated samples and the FE analysis are carried out in order to elucidate which parameter describing the pore population (volume, projected area, distance from the surface …)

seems predominant in terms of fatigue harmfulness.

10:25 AM

In-situ Measurement of Lattice Strain in Al-Li Alloys: *Armand Beaudoin*[1]; Mark Obstalecki[2]; Wesley Tayon[3]; Ulrich Lienert[4]; Peter Kenesei[4]; [1]University of Illinois at Urbana-Champaign; [2]Cornell University; [3]NASA; [4]Argonne National Laboratory

Far-field High Energy Diffraction Microscopy provides the capability to query crystallographic orientation and elastic strain within the sample volume of a polycrystalline material. This technique has been applied to the in situ loading of Al-Li alloys at beamline 1-ID of the Advanced Photon Source of Argonne National Laboratory. The spatial arrangement of several pancake-shaped grains in a tensile sample is determined through a combination of in situ and ex situ techniques. In situ diffraction data is coordinated with simulation to detail the elasto-plastic transition on a grain-by-grain basis. While full 3D realization of the microstructure is not recovered in the present program, agreement between lattice strain data taken in the constrained environment of the sample interior with an idealized 3D simulation lends considerable insight into material performance. Techniques aiding examination of microstructure for a production heat-treatable aluminum alloy, such as use of the conical slit cell, will also be discussed.

10:45 AM

Numerical Simulation and Experimental Analysis of Notched Failure Processes in Composite Laminates: *Ian Sinclair*[1]; Qingda Yang[2]; Mark Mavrogordato[1]; Brian Cox[3]; Mark Spearing[1]; [1]University of Southampton; [2]University of Miami; [3]Teledyne Scientific

The incidence of complex, multiple cracking events at stress concentrations is well recognised in fibre reinforced laminates. Recent advances in numerical methods, such as extended and augmented finite element modelling (X-FEM and A-FEM respectively) provide significant opportunities to address such failure processes in an efficient and mechanistically meaningful manner. X-ray computed tomography (CT) provides vital model initialisation and validation input to such simulation efforts, with the present paper investigating: (a) in situ synchrotron CT analysis of damage evolution from a notch in carbon fibre epoxy composites of three matrix toughness levels, (b) corresponding A-FEM simulations based on careful material property calibrations, and (c) comparison and discussion of experimental and simulation results in relation to crack initiation, propagation and damage coupling processes.

11:05 AM Break

11:20 AM

3D Image-based Modeling of Residual Stresses in Hybrid Shape Memory Alloy / Ceramic Composites: Brian Lester[1]; Yves Chemisky[1]; Dimitris Lagoudas[1]; Richard Everett[2]; Siddiq Qidwai[2]; *Andrew Geltmacher*[2]; [1]Texas A&M University; [2]Naval Research Laboratory

The capability of Shape Memory Alloys (SMAs) to generate a residual stress state in a hybrid SMA-ceramic composite for extreme environments is explored here. It is advantageous to generate a compressive residual stress in ceramic phases for improved mechanical behavior, such as fatigue crack initiation. SMA-MAX phase composites with heterogeneous, irregular microstructure are considered. 3D image-based modeling is used to simulate the effect of simple thermo-mechanical loading paths on the resulting residual stresses in the MAX-phase. X-ray tomographical data is used as direct input in finite element models. A recent phenomenological model for the constitutive behavior of SMAs is then used to describe the response of the SMA phase while an elastic-plastic constitutive law is used for the MAX phase behavior. It is shown that using isobaric loading paths, martensitic transformations in the SMA generate irrecoverable strains in the ceramic phase which results in compressive residual stress state upon unloading.

11:40 AM

Integrated Experimental and Simulation Approaches for Mesoscopic Deformation of Polycrystalline Metal: Crystal Plasticity FEM: *Yoon Suk Choi*[1]; Michael Groeber[2]; Paul Shade[2]; Todd Turner[2]; Jay Schuren[2]; Michael Uchic[2]; Christopher Woodward[2]; Dennis Dimiduk[2]; Triplicane Parthasarathy[1]; [1]UES, Inc.; [2]Air Force Research Lab.

Understanding the microscopic origins and evolution of damage and plastic instability, via crystal plasticity FEM (CP-FEM) remains a focus of the materials property modeling community. Previous studies show that validation of CP-FEM approaches for polycrystals both in global and mesoscopic scales will benefit from emerging new experimental and characterization schemes. Advanced controlled micro-mechanical testing capabilities allow experimental testing at the same scales that are amenable to simulation and, at the same time advanced 3D data reconstruction and microstructure analysis enables mesoscopic simulations having fully informed 3D geometries. In the present study, such integrated experimental characterization and simulation via CP-FEM were used to investigate both global and mesoscopic plastic responses of polycrystalline samples. Preliminary parametric studies including the optimization of the simulation geometry and boundary conditions are discussed. Simulation results from those optimized conditions are compared to experiment and analysis results in 2D and 3D both at global and mesoscopic scales.

Microstructure-Property Relationships in 3D: Characterization and Simulation

Tuesday AM — Room: Sunburst
July 10, 2012 — Location: Seven Springs Mountain Resort

9:45 AM

Twin Connectivity in Wrought Magnesium Alloys: Matthew Barnett[1]; Alireza Ghaderi[1]; *Mark Nave*[1]; [1]Deakin University

When a fine-grained magnesium alloy yields by twinning, a plateau is observed in the stress-strain curve. This "yield elongation" decreases and eventually disappears with increasing grain size. Optical microscopy and electron backscatter diffraction (both 2D- and 3D-EBSD) were used to investigate twin connectivity across grain boundaries in wrought magnesium specimens with varying grain sizes. Twin connectivity was found to increase with decreasing grain size and there was good strain compatibility between connecting twins. Based on these results, it was proposed that twinning occurs via an autocatalytic process whereby a twin in one grain nucleates one or more twins in another grain and that twinning spreads throughout the material as this process repeats itself. A simple mathematical description of this theory was used to calculate the minimum twin connectivity for the appearance of the yield elongation and this value was in good agreement with the experimental results.

10:05 AM CANCELLED

The Influence of 3D Networks of Aluminides on the Strength of Al-Si Piston Alloys: *Guillermo Requena*[1]; Zahid Asghar[1]; [1]TU Vienna

The 3D architecture of multicomponent Al-Si piston alloys is studied by synchrotron microtomography as a function of the solution treatment time. The presence of eutectic Si, Ni, Cu and Fe results in the formation of hybrid 3D structures of aluminides and Si that improve the strength of the alloys by a load transfer mechanism from the Al-matrix to the highly interconnected rigid networks. Cu-containing Al-Si alloys show the presence of Al2Cu, Al7Cu4Ni, Al4Cu2Mg8Si7 and AlSiFeNiCu aluminides that result in a larger interconnectivity of the 3D networks than in the case of Cu-free Al-Si alloys. The load carrying capability of the different aluminides and of the network formed by eutectic Si and aluminides is correlated with their 3D morphology. The preservation of interconnectivity and, up to some extent, of the morphology of the rigid phases during solution treatment is governed by the degree of contiguity between aluminides and Si.

10:25 AM

Measurements of Materials During In-situ Experiments Using X-ray Tomography: *Brian Patterson*[1]; Kevin Henderson[1]; Robert Gilbertson[1]; Christopher Hamilton[1]; Kimberly Obrey[1]; Nickolaus Smith[1]; [1]Los Alamos National Laboratory

During most of the time x-ray computed tomography (CT) has been practiced, it has been limited to generating 'pretty', albeit useful pictures of materials. These 3D images give scientists a qualitative understanding of the sample morphology. Scientists have begun to take this data one step further and added the ability to quantify void sizes, shapes and their distributions. Coupling this with an in-situ cell such as tension, compression, tearing, or heating, now it is possible to quantifiably measure how these features change as a result of response to dynamic change. It is possible to quantifiably measure and compare changes as a result of age, or some induced stress. We will discuss our recent work with polymers and metals using a compression/tension load cell within a micro-CT instrument. We will demonstrate differences not seen qualitatively, can be measured quantitatively as a method to compare lot-to-lot or experiment-to-experiment variations.

10:45 AM

Development of Fully Automated Serial-sectioning 3D Microscope and Topological Approach to Pearlite and Dual-phase Miscrostructure in Steels: *Yoshitaka Adachi*[1]; Naoko Sato[1]; [1]Kagoshima University

Using a newly developed fully-automated serial sectioning 3D microscope "Genus_3D" and a conventional dual beam SEM, we examined ferrite-martensite dual phase and eutectoid pearlite microstructures with a particular attention to topology and differential geometry. Genus, Euler characteristics, Gaussian curvature and mean curvatures were obtained from 3D reconstructions. A variation of martensite morphology in DP steel, in particular, connectivity was examined, which was applied to understand enhanced internal stress partitioning in ferrite surrounded by honeycombed martensite and fracture mechanism. In addition, morphological variation of lamellar cementite in pearlite during spheroidizing treatments was investigated in 3D. This 3D observation revealed that there were a lot of holes and fissures in cementite lamellae, which potentially accelerates the spheroidizing. The lamellar structure disintegration into particles was discussed from surface area change per unit volume and local surface morphology, i.e. curvature.

11:05 AM Break

11:20 AM

Quantification of Primary Phase Undercooling of Rapidly Solidified Droplets with 3D Microtomography: Arash Ilbagi[1]; Pooya Delshad Khatibi[1]; *Hani Henein*[1]; Charles-Andre Gandin[2]; Dieter Herlach[3]; [1]University of Alberta; [2]MINES ParisTech & CNRS, CEMEF UMR; [3]c/o Institute of Materials Physics in Space, DLR

Powders of different compositions of Al-Fe and Al-Cu alloys were atomized and the microstructure of the atomized droplets were examined using X-ray micro-tomography. A method was developed to remove X-ray artifacts and background noise from the particles images. The method developed involves creating a clean mask file using MATLAB image toolbox, followed by applying the mask file to the original image to achieve clean images for the particle of interest. The effect of cooling gas and particle size on the microstructure and volume percent of porosity and its distribution within droplets were investigated using a 3D software, AVIZO. Separate features of interest in the droplets, such as region of initial growth and primary dendrites, were investigated at the various stages of solidification. The data is used to estimate the primary phase undercooling of the droplets. The trends in this data with respect to atomization processing conditions will be discussed.

11:40 AM

Using Combined EBSD/EDS to Characterise Nickel-based Superalloys in 3D: *Geoff West*[1]; Rachel Thomson[1]; Daniel Child[1]; [1]Loughborough University

An automated methodology for collecting simultaneous 3D Electron Backscatter Diffraction (EBSD) and Energy Dispersive Spectroscopy (EDS) data is described that has successfully been used to study the phase connectivity in nickel based superalloys. 3D EBSD/EDS data collection has been undertaken in random areas of bulk materials and at site-specific microstructural features using an insitu liftout procedure within the dual beam microscope. The site-specific locations include at a crack tip in a fatigue sample and at a surface degraded by corrosion. The applicability of the technique to characterise other systems will also discussed.

12:00 PM

The Influence of Microstructure on 3D Crack Morphologies in a New Naval Steel: *Marie Cox*[1]; David Rowenhorst[2]; Richard Fonda[2]; [1]National Research Council Postdoctoral Fellow; [2]U.S. Naval Research Laboratory

The complex 3D shapes of fatigue cracks are difficult to accurately characterize by surface (2D) observations, especially when at the early stages of fatigue crack growth where the morphology of the crack is heavily influenced by the material microstructure. We will discuss the effect of microstructure on the 3D crack morphology of region 1 fatigue cracks in a high-strength low-alloy naval steel (HSLA-115). To determine the salient features that affect the crack path, including microstructural morphology and crystallographic orientation, EBSD and optical microscopy are used to characterize the material near the crack. These salient features are then compared to the 3D crack morphology obtained from x-ray tomography, thereby determining crack resistant features, indicating the processing parameters that improve fatigue crack resistance in this steel and providing accurate 3D crack morphology input for predicative models.

Poster Session 2: Image Processing, Digital Representations of 3D Microstructures, and Applications of 3D Experimental Techniques

Tuesday PM	Room: Exhibit Hall
July 10, 2012	Location: Seven Springs Mountain Resort

P2-01: 3D Characterization and Reconstruction of the Primary Austenite Dendrite and Interdendritic Space in Lamellar Cast Iron: *Attila Diószegi*[1]; Ruben Lora[1]; Vasilios Fourlakidis[2]; Guillem Prats Vilaseca[1]; Álvaro Díaz de Aguilar[1]; [1]Jönköping University; [2]Swerea Swecast AB

The presented investigation focuses on the morphology of austenite dendrites in lamellar cast iron solidified under different cooling conditions. Using a sequential investigation scheme including colour etching, image analysis and invoking stereological relations, it has been demonstrated that 3D geometrical parameters of the dendrite network can be approximated using 2D observations. The volume fraction of a primary dendrite is approximated by its area fraction and the primary dendrite envelope is approximated by the perimeter of the dendrite phases observed on 2D micrographs. Longer solidification times result in smaller dendrite envelopes while the precipitated primary phase remains independent of the cooling rate. The approximated hydraulic diameter of the space between dendrites indicates a larger interspace between dendrites when the solidification time is long. 3D solid models of the primary austenite dendrites are created, opening the opportunity for computational fluid dynamics (CFD) calculations.

P2-02: 3D Characterization of Damage within Copper using Micro and Nano X-ray Tomography: *Brian Patterson*[1]; Kevin Henderson[1]; Ellen Cerreta[1]; J Escobedo-Diaz[1]; Darcie Dennis-Koller[1]; [1]Los Alamos National Laboratory

Laboratory based x-ray micro computed tomography (micro-CT) with the addition of a full measuring package, can lend measurements and statistics of voids within damaged materials that traditional 2D microscopy cannot. Micro-CT is used to image these materials and quantitatively measure the specimens' voids; their sizes, shapes, and distributions. Micro-CT also images the connectivity of voids, which may not be apparent in 2D. Damage studies of impacted copper at the incipient spall stage at various impact profiles will be shown. Additionally, sub-micrometer voids can be imaged using 3D nanoCT (resolution ~150 nm) which can also be quantified for shape and size. At this high resolution void surface facets can be imaged as the voids grow against copper grains. Comparisons between 2D microscopy will be shown highlighting the strength of this technique.

P2-03: 3D Characterization of High Burn-up MOX Fuel: *Melissa Teague*[1]; Jessica Riesterer[1]; Brian Gorman[1]; Michael Tonks; Michael Tonks[1]; [1]Idaho National Laboratory

The increasing demand for cost effective green energy has led to a renewed interest in nuclear energy, including the commercialization of fast breeder reactors (FBR's). Currently fast reactor performance is largely defined by the limitations of the materials involved in reactors, especially the metallic or mixed oxide ((U, Pu)O2) fuel itself. Problems include fission gas generation, changes in thermal conductivity, microstructure changes within the fuel, fuel swelling, and fuel cladding chemical interaction (FCCI). Due to the highly radioactive nature of spent fuel, novel block lift out techniques are required for collecting chemical and structural information. Results from the utilization of a dual-beam FIB along with EDS and EBSD detectors to analyze the 3D structure of high burn-up MOX fuel will be presented.

P2-04: 3D Identification of Inclusions in NiTi Alloy after Electropolishing: *Tadeusz Hryniewicz*[1]; Ryszard Rokicki[1]; [1]Politechnika Koszalinska

The aim of the paper is 3D investigation of inclusions appearing on surface of NiTi alloy after electropolishing operations. Equiatomic NiTi alloy is characterized by unique properties, including superelasticity and shape memory, that make it very attractive for biomedical applications. It is well known that NiTi requires controlled processing to achieve optimal mechanical and thermal properties. In the studies of NiTi multiple inclusions appeared on the surface after electropolishing. Scanning electron microscope Phenom G2 Pro was used to observe the inclusions. 3D images have been obtained, mostly of rectangular shape, with the dimensions of the inclusions changing from below a micrometer up to 15 micrometers in height, and respective widths and lengths. Occuring on the surface jetting characteristic with lowering the matrix around the grain results generally from the electrolyte motion during the process of electropolishing. The inclusions surely affect the biocompatibility of the NiTi alloy if used as biomaterial.

P2-05: Advances in 3D Imaging and Analysis of Materials Using Electron and Ion Beams: *Hans Fleurkens*[1]; Daniel Phifer[1]; [1]FEI Company

Serial sectioning using precise FIB milling and high resolution electron imaging is an established technique to produce data sets used to reconstruct samples in 3D. Typically data collection has been done with a single image capture of information from each serial slice. The ability to collect multiple images from the same slice allows using optimized settings for capturing all information (like topographic, compositional data as well as data for crystallographic and chemical analysis) from the same sample that can be used for in-depth analysis. Huge improvements have been made in controlling stability and drift of this process allowing the analysis of larger volumes at high resolution. This also applies to traditionally more difficult non-conductive or partially conductive samples by using a unique method that combines high vacuum milling with low vacuum imaging.

P2-06: Automated Segmentation and Characterization of 2D/3D Fibrous Composite Optical Micrographs using the Hough Transform: *Craig Przybyla*[1]; [1]Air Force Research Laboratory

Micrographs of fibrous composites can be difficult to segment and characterize because of the challenge of identifying the individual fibers when they are touching or when the contrast between the fibers and other constituents (e.g., matrix) is minimal. In this work, circle and elliptical Hough transforms are used to identify the individual fibers in a SiC/SiC ceramic matrix composite where there is little or no contrast between the individual fibers and the matrix. Techniques are used to reduce the dimensionality of the elliptical Hough transform to reduce the memory requirements of the algorithm. Once the fiber locations are known, the fiber statistics can be calculated including the correlation statistics which describe spatial relationships (e.g., clustering) between the fibers and the fibers and the other constituents. Implications of these techniques will also be considered relative to the development of methods to reconstruct, segment and characterize 3-dimensional datasets obtained via serial sectioning.

P2-07: Development of a Data Fusion Module to Register and Combine EBSD, EDS, and Electron-optic Images: *Megna Shah*[1]; Michael Uchic[2]; Michael Groeber[2]; [1]UES, Inc.; [2]Air Force Research Laboratory

Modern electron-optic-based serial sectioning instruments can collect a suite of multi-modal data at each section—images, electron backscatter diffraction (EBSD) and energy dispersive x-ray spectroscopy (EDS) maps, and other data types. While it is possible to collect some data simultaneously, it is often advantageous to collect data serially in order to optimize both data quality and spatial frequency. In practice, the suite of data is usually subject to some distortions with respect to each other. The focus of this work is to develop a generic framework to correct distortions, register and fuse a suite of multi-modal data in order to more fully characterize a microstructure and assist with segmentation. Combining EBSD and EDS data streams with higher resolution images allows for faster, more accurate determination of all phases and grains in the microstructure. Using a Ni superalloy as an example, we will describe and apply the data fusion module.

P2-08: Digital Representation Environment for the Analysis of Microstructure in 3D (DREAM.3D): *Michael Groeber*[1]; Michael Jackson[2]; [1]AFRL; [2]BlueQuartz Software

DREAM.3D is an open and modular software environment that allows users to reconstruct, instantiate, quantify, mesh, handle and visualize microstructure digitally. It is being developed by the Air Force Research Laboratory in conjunction with a host of collaborators from Carnegie Mellon University, the Naval Research Laboratory, Ohio State University, Los Alamos National Laboratory, and others. This poster will present the architechure of the environment along with the current functionalities. This poster is meant to educate the community on the existing state-of-the-art tools and build a developers network for advancing these tools in the future.

P2-09: FIB/SEM Tomography as a Tool to Study Bulk Membrane Recycling in Central Synapses: *Liubov Belova*[1]; Oleg Shupliakov[2]; [1]KTH, Royal Institute of Technology; [2]Karolinska Institute

Many physiological studies proposed that bulk membrane endocytosis is used during increased neuronal activity to recover synaptic vesicles in synapses in CNS. During this cellular process large membrane compartments detach from the plasma membrane and endosomes are formed to be gradually transformed into synaptic vesicles. Large size of these synapses allows for microinjections of different compounds, which perturb protein-protein and protein-lipid interactions selectively during the synaptic vesicles cycle. Currently, conventional TEM is routinely used to analyze ultrastructural effects of the microinjected compounds. This approach does not allow analysis of large areas of axons, which is desirable for detailed analysis of the concentration dependent morphological effects in synapses at different distances from the site of microinjection. In this study we aim at improving the use of the lamprey giant synapse by applying the FIB technology in combination with scanning electron microscopy, which allows for screening of large tissue volumes in 3D.

P2-10: 3D Analysis of Phase Separation in Ferritic Stainless Steels: Joakim Odqvist[1]; Jing Zhou[1]; Wei Xiong[1]; *Peter Hedström*[1]; Mattias Thuvander[2]; Malin Selleby[1]; John Ågren[1]; [1]KTH (Royal Institute of Technology); [2]Chalmers University of Technology

The embrittlement of ferritic stainless steels during low temperature aging is attributed to the phase separation with Fe and Cr demixing. The nano-scale of the decomposed structure with only minor compositional fluctuations and short distances between the enriched and depleted regions has been a challenge for developing next generation advanced steels with high performance. A wide selection of experimental and modeling tools have been used to try and quantify these types of structures. These analyses often focus on rather late stages of decomposition where the mechanical properties are already seriously affected. The recent advances in 3D tools like phase-field and atom probe tomography have created a need for good quantitative procedures of evaluating the structure and also to link results from the continuum approach to the individual atom measurements. This work aims at addressing this need.

P2-11: Generation of Micro-Architectures: Philippe Young[1]; David Raymont[1]; Liang Hao[1]; *Kerim Genc*[2]; [1]University of Exeter; [2]Simpleware Ltd.

Internal micro-architectures have many uses such as light-weight support structures, bone substitutes, scaffolds as well as aiding bone-implant integration. Designing such structures using traditional CAD software is non-trivial. Micro-architectures can be generated to conform to an existing domain, specified either by a CAD model or by a volume acquired using 3D imaging techniques such as CT, micro-CT and MRI. The technique developed by the authors relies on working in image-space to ensure the robustness of operations and to take advantage of image-based meshing for any computational analysis. Micro-architectures of specific volume fractions are generated using a re-iso-surfacing technique. The authors introduce the concept of a relative density map, a method for representing the desired relative densities in the micro-architecture. Examples are given of functionally graded and arbitrary graded structures in both 2D and 3D. The advantages of an image-based approach are demonstrated for the ease of generating volume meshes.

P2-12: Handling Misalignment and Drift in 3D EBSD Data Sets: Yuchi Huang[1]; *Brandon Laflen*[1]; Andrew Deal[1]; Ian Spinelli[1]; Anthony Barbuto[1]; Timothy Hanlon[1]; [1]GE Global Research

GE Global Research is exploring the 3D reconstruction of high temperature materials to understand material behavior in lifing applications. Large volumes of material are required to generate the appropriate statistical understanding of grain morphologies, grain boundary types and distributions, and residual plastic strain. Consequently, GE has adopted mechanical sectioning coupled with EBSD analysis as the methodology for investigating regions of interest. Among the major factors that affect the accuracy of such a reconstruction are thermal or mechanical drift during EBSD measurements and the precision and accuracy of sample alignment. To correct for these unavoidable issues when reconstructing the final volume, an algorithm based on grain center-of-mass and additional shape factors has been developed and applied to a data set. Results show a significant improvement in slice-to-slice registration.

P2-13: High Energy Diffraction Microscopy as a Tool for High Pressure Research: *Joel Bernier*[1]; Nathan Barton[1]; Donald Boyce[2]; Daniel Farber[3]; [1]Lawrence Livermore National Laboratory, Engineering Technologies Division; [2]Cornell University, Sibley School of Mechanical and Aerospace Enginering; [3]Lawrence Livermore National Laboratory, Condensed Matter and Materials Division

The marriage of high energy diffraction microscopy (HEDM) and the diamond anvil cell has the potential to revolutionize experiments in high pressure physics. The 3-dimensional nature of the measurements alleviate the ambiguity in the non-hydrostatic component of the applied stress, enable determination of parent/product orientation relationships and preferred variant selection for phase transformations and/or twinning, and provide enough data to perform detailed structure refinement even for heavily deformed materials. Unit cell volumes can also be determined to very high precision, which is critical to accurate equation of state (EOS) measurements. This technique was recently used to demonstrate preference of the Burgers mechanism for the α->ε phase transition in iron at quasi-static rates, something simply not possible via other methods. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

P2-14: In-situ Investigations of the Interface Dynamics of Materials using Ultra-fast X-ray Tomographic Microscopy and Laser Heating: *Julie Fife*[1]; Peter Voorhees[2]; Marco Stampanoni[3]; [1]Paul Scherrer Institut; [2]Northwestern University; [3]Paul Scherrer Institut and ETH and University of Zurich

Non-destructive synchrotron X-ray tomographic microscopy at the TOMCAT beamline of the Swiss Light Source is ideal for studying the dynamics of many materials systems in real time, and particularly well-suited for in-situ coarsening in Al-Cu systems [1-3]. Coupling the recently-commissioned ultra-fast data acquisition endstation [4] with the newly-developed laser-based heating system [5] provides an unprecedented environment for observing and characterizing the dynamics of formation and growth in materials at elevated temperatures. For instance, in the range of 400-1700°C, a full data set with several hundred projections over 180° can be captured in less than 1s. This talk presents results on early-stage coarsening in Al-Cu alloys, now observable because of the above-mentioned improvement in temporal resolution. Specifically, we focus on characterizing interface velocity and its relation to morphological features such as interface curvature. We also discuss the impact of these initial changes on the later stages of microstructural evolution. [1] L.K. Aagesen, et. al., Nature Physics, 6, 796-800, 2010. [2] L.K. Aagesen, et. al., Acta Materialia, 59, 4922, 2011. [3] L.K. Aagesen, et. al., Scripta Materialia, 64(5), 394-397, 2011 [4] R. Mokso et al., AIP Conf. Proc. 1234, SRI2009 (2010) [5] JL Fife et al., J. Synchrotron Rad, submitted.

P2-15: In-situ Tomographic Imaging of 3D Microporous Composite Anode of Lithium-ion Batteries: *XIanghui Xiao*[1]; Fikile Brushett[1]; Lynn Trahey[1]; John Vaughey[1]; [1]Argonne National Laboratory

Over the past decade different alternative higher capacity anodes have been proposed to replace graphitic carbon anodes, which are utilized in most commercially-available batteries but have relatively low energy storage capacity. However, the main challenge to the alternative anode materials is the short working lifetime due to significant volume change during operation. In this work we have applied synchrotron micro-tomography to a type of 3D microporous composite anode and monitored changes in anode structure in situ and in real time. From the results we are able to track the topological structure changes in the anode and calculate the surface-volume ratio evolution along with the cycling. Such information is not only helpful to improve the engineering of the 3D microporous composite anodes but also offers critical insights into the structure-activity relationships of high capacity porous materials within operating electrochemical energy storage devices.

P2-16: Optimizing Scholastic Process for Efficient Microstructure Reconstruction: *Seun Ryu*[1]; Dongsheng Li[1]; [1]Pacific Northwest National Laboratory

Large microstructure with high resolution was reconstructed by data reduction, fusion and reconstruction. Information from multiple images with different resolution was used in data fusion. Images obtained at different resolution, different locations were reduced using statistical correlation functions. The structure information was fused together to reconstruct a high resolution large domain image. Reconstruction was performed using different methods, stochastic, Gaussian filter method and hybrid methods. Different cooling schedules in simulated annealing were utilized and compared. Genetic algorithm is also implemented in reconstruction. Dramatic increase of computation efficiency has been achieved in image fusion and reconstruction.

P2-17: Investigating Shock Damage in Polycrystalline Cu through High-Energy Diffraction Microscopy: *John Bingert*[1]; R.M. Suter[2]; J. Lind[2]; S.F. Li[2]; C.M. Hefferan[2]; C.P. Trujillo[1]; [1]Los Alamos National Laboratory; [2]Carnegie Mellon University

The relationship between microstructure and shock damage is critical to understand the response of materials to dynamic loading states, enabling the development of predictive damage models and damage-tolerant materials. For this investigation, high-energy diffraction microscopy (HEDM) at the Advanced Photon Source at Argonne National Laboratory was used to non-destructively characterize an annealed polycrystalline Cu sample in both its pre-shock and post-shock states. Shock loading entailed the development of a plate-on-plate impact technique suitable for soft-capturing the sub-size (1.2 mm diameter x 0.8 mm long) pre-characterized sample. After ex situ impact, tomography measurements revealed a region of incipient spallation voids distributed across the sample's mid-plane. Subsequent HEDM thus permitted unprecedented direct correlation between 3D microstructure of a bulk sample and damage evolution, with the definitive identification of spall initiation sites. Issues regarding diffraction pattern indexing in the deformed state, registration between states, and HEDM data interpretation will be addressed.

P2-18: Investigation of the 3D Grain Size and Shape of WC in Cemented Carbides: *Ali Gholinia*[1]; Bartlomiej Winiarski[1]; Philip J. Withers[1]; Ida Borgh[2]; Peter Hedström[2]; Joakim Odqvist[2]; Annika Borgenstam[2]; Ken Mingard[3]; Mark G Gee[3]; [1]University of Manchester; [2]KTH Royal Institute of Technology; [3]National Physical Laboratory

Cemented carbides consist of hard tungsten carbide (WC) grains embedded in a ductile Co-rich binder phase. The mechanical properties are largely depending on the grain size of WC, which will increase during production, i.e. sintering. A numerical model has been developed to predict the grain growth of WC. The grain size has so far been evaluated from 2D sections using electron backscattered diffraction (EBSD) and the 3D size distribution has been calculated using an inverse Saltykov method. However, experimental verification is necessary and thus direct 3D measurements are required. In this work 3D-EBSD is used to evaluate both the 3D size and prismatic shape of WC grains. The 3D measurements are compared to the estimations from 2D sections and the implication of the new findings on the grain growth model is discussed.

P2-20: Micro-computed Tomography, a 3D Tool for Non-destructive Visualisation and Analysis: *Evi Bongaers*[1]; Remy Van den Bosch[2]; [1]SkyScan N.V.; [2]University of Antwerp

Micro-computed tomography (micro-CT) is a powerful technique to visualize and measure the internal microstructure of various materials, both biological as non-biological, in a non-destructive way. As an example, this talk will focus on the use of micro-CT in the study of pores and pore networks in rocks for oil exploration. The resulting dataset of micro-CT is a set of thin, virtual slices through the object. 3D analysis software can extract unique numerical characteristics, such as internal porosity, size distribution for pores or grains, etc. Visualization software shows a realistic 3D object on the screen. This gives possibilities for virtual sectioning, and creating movies of flights around and inside the object. Micro-CT has an added value and can provide new information in 3D, leading to new insights in materials and processes. In addition, it can be combined with additional stages (temperature, pressure,…) for dynamic studies of microstructural behavior.

P2-21: Multi-scale Homogenisation for 3D Microstructures: Philippe Young[1]; David Raymont[1]; Liang Hao[1]; *Kerim Genc*[2]; [1]University of Exeter; [2]Simpleware Ltd.

Synthetic and natural micro-architectures (e.g. foams, bone, etc.) are becoming increasingly popular for applications requiring tailored material properties. The method developed by the authors enables the bulk response of large inhomogeneous domains with distinct length-scales to be obtained through characterisation. The characteristics obtained from the process can also be visualised to highlight the variation of properties. By considering independent sub-volumes the characterisation technique provides a high degree of parallelism and considerably reduced memory requirements. The technique can be applied to natural structures such as in the generation of a macro model of the femur using results obtained from mechanical simulations of trabecular bone at a micro level. Effective properties obtained using the developed methods are shown to be in good agreement with those obtained using kinematic uniform boundary conditions (KUBC).

P2-22: Study of Three Dimensional Microstructural Morphologies of Dendritically Solidified Alpha-Mg(X): *Mingyue Wang*[1]; Tao Jing[2]; [1]Tsinghua University & Arizona State University; [2]Tsinghua University

Magnesium has a hexagonal close-packed (h.c.p.) structure, as a result, some new issues appeared. Indeed, it is very unclear to date about how to describe theoretically the morphologies, orientation selection and evolution mechanism of h.c.p. dendrites. The main objective of the present study is to establish a fundamental understanding of the 3D morphologies and orientation selection of dendritic primary a-Mg solid solution phases. In order to elucidate this question, Mg-Al, Mg-Zn and Mg-Sn binary alloys were selected. The present work are principally foused on studying 3D morphologies characteristics of a-Mg primary dendrite phases formed within the alloy melts with a combination of experimentally 3D X-ray tomography technique and computationally phase-field simulations of equiaxed dendritic growth and directional freezing of magnesium alloys. It includes three main axes.

P2-23: Three Dimensional Composition Mapping of a White Spot VAR Defect in Nickel Alloy 718: *Trevor Watt*[1]; Eric Taleff[1]; [1]The University of Texas at Austin

A Niobium-deficient "white spot" in a vacuum arc remelted (VAR) ingot of Nickel-based Alloy 718 is studied using three-dimensional data sets. Optical microscopy, electron microscopy, and X-ray fluorescence energy dispersive spectroscopy (XRF-EDS) are used, in concert with serial polishing, to generate feature and composition data in three dimensions. Accurately measuring local chemical composition over a large volume with existing EDS technology can take a prohibitively long time. To overcome this issue, a combination of low-accuracy elemental area maps and high-accuracy spot scans is investigated. This approach produces accurate composition data for select features, while maintaining reasonable data acquisition times. Details and results of this procedure are presented. Implications of the resulting three-dimensional data on understanding the formation and evolution of white spots in nickel-based superalloys are discussed.

P2-24: Three Dimensional Segmentation and Reconstruction from Serial Micrographs of Powder Metallurgy Polycrystals: *Michael Marsh*[1]; Laurent Bernard[2]; Murali Gorantla[3]; Yoon Suk Choi[3]; [1]Visualization Sciences Group; [2]Noesis; [3]UES

High resolution microscopy enables the microstructural study of polycrystalline metals and intermetallics. We report the experimental and image processing details of our solution to identify grain boundaries and reconstruct the 3D grain network of powder metallurgy Ni-base superalloys. We were able to observe and record serial micrographs covering a significant 3D volume at high spatial resolution by using the automated iterative polishing and microscopy of the Robo-Met.3D(TM) serial sectioning system. The contrast in the micrographs clearly revealed grain boundaries by visual inspection, but there were inter- and intra-granular inclusions. Because the grayscale intensity of the inclusions was indistinguishable from the grain boundaries, normal software methods could not be used to segment the grains. We applied image smoothing and morphology operators to differentiate the inclusions from the grain boundaries. We show the full 3D reconstruction of the grain network and discuss the 3D microstructural characteristics of powder metallurgy Ni-base superalloys.

P2-25: Tracking Geometrical Features using Near-field High Energy X-ray Diffraction Microscopy: *S. F. Li*[1]; J. Lind[2]; C. M. Hefferan[2]; A. D. Rollett[2]; R. M. Suter[2]; [1]Lawrence Livermore National Lab; [2]Carnegie Mellon University

Near-field High Energy X-ray Diffraction Microscopy (HEDM) is one of a handful of non-destructive and spatially resolved volumetric orientation imaging techniques currently available for polycrystalline materials. Recent developments of HEDM reconstruction algorithms have led to significant improvements in our measurement capabilities. Combined with work in geometrical extraction and tracking, we are now able to follow thousands of grains and boundaries, often with extremely complex dynamics across multiple anneal states. In this talk, we will present some of our recent advances, namely in orientation reconstruction and geometrical tracking. Error estimation and propagation will also be discussed in the context of geometrical extraction from 3D X-ray data. Example applications of our analysis methods to grain coarsening and plastic deformation will also be presented.

P2-26: X-ray Micro-Laue Diffraction in 3D at the Canadian Light Source: *Renfei Feng*[1]; [1]Canadian Light Source

Canadian Light Source is the only national synchrotron facility in Canada. VESPERS beamline is a bending magnet based hard X-Ray microprobe beamline capable for 3D Laue diffraction. Differential Aperture X-Ray Microscopy (DAXM) was implemented by combining wire-scan with sample-scan to provide unique non-destructive analytic technique. Depth-resolved diffraction images can be created from this technique. Therefore, three-dimensional crystal orientation and strain distribution can be obtained. Beamline is equipped with a specially designed double crystal and double multilayer monochromator, and is capable to provide the beams with widely differing bandwidths of 0.01%, 1.6%, 10%, and polychromatic beam, over the energy range of 6-30 keV. Beamline is in operational since 2008, and DAXM is available since 2010. Beamline design, endstation capabilities, and a few case studies will be presented.

P2-27: Characterization of Carbonate Rocks through X-ray Microtomography: Debora Pilotto[1]; Sérgio da Fontoura[1]; *Sidnei Paciornik*[2]; Marcos Henrique Mauricio[1]; [1]PUC-Rio; [2] PUC-Rio

Image characterization of rocks is generally carried out by optical and scanning electron microscope techniques. In this paper µCT was used in order to obtain microstructural parameters. The experimental program consisted in obtaining these properties from three different carbonate rocks: the Roman, Turkish and Itaboraí Travertines, selected since they possess similar properties to the Brazilian oil-bearing pre-salt rocks. The results have shown that µCT is very useful in determining the porosity and pore size distribution, as compared to traditional porosimetry methods, establishing the pore arrangement within the rock matrix and detecting their connectivity. Additionally, the generation of 3-D models allowed a faithful representation of the samples and allowed the selection of regions for thin section preparation of their most representative features, which were then analyzed by Digital Optical Microscopy.

P2-28: Characterization of Pores and Cracks in Underwater Welds by µCT and Digital Optical Microscopy: *Sidnei Paciornik*[1]; Timo Bernthaler[2]; Valter dos Santos[3]; Mauricio Monteiro[3]; Marcos Henrique Mauricio[3]; Alexandre Bracarense[4]; Ezequiel Pessoa[5]; [1] PUC-Rio; [2]Hochschule Aalen - Technik und Wirtschaft; [3]PUC-Rio; [4]UFMG; [5]CEFET-MG

Underwater shielded metal arc wet welding with coated electrodes is a common procedure for in situ repair of structural parts of offshore oil production units. However, there are serious difficulties in obtaining sound welds similar to the ones achieved under atmospheric conditions. The water environment surrounding the weld pool is usually responsible for very high cooling rate and high hydrogen content in the weld metal. These factors may lead to the formation of porosity and cracks in the weld metal which are not precisely analyzed through the conventional 2D techniques. The 3D visualization and measurement of these defects can contribute significantly to a better characterization and prediction of weld metal properties. In the present work wet welded steel samples were analyzed by µCT and Digital Optical Microscopy, with the aim of measuring, both in 2D and 3D, the concentration, size and shape of pores and cracks.

Digital Representation of 3D Microstructures

Tuesday PM	Room: Exhibit Hall
July 10, 2012	Location: Seven Springs Mountain Resort

6:30 PM Invited

Storage and Sharing of Large 3D Imaging Datasets: Richard Boardman[1]; *Ian Sinclair*[1]; Simon Cox[1]; Philippa Reed[1]; Kenji Takeda[1]; Jeremy Frey[1]; Graeme Earl[1]; [1]University of Southampton

The scientific and engineering communities are investing in the generation large voxel datasets. Procedures and standards to record acquisition, sample condition, processing algorithms and imaging parameters are vital to maintain long-term data value. Even when these are conserved, data remains largely inaccessible to the wider community, hindering both business and research exploitation, an issue increasingly recognised by funding bodies. Engaging imaging communities in the use and development of standards-compliant schemas and ontologies is therefore essential. Tools to then conserve significant volumes of 3D data are discussed, including Cloud compute and storage opportunities. Policy and practical issues are considered in relation to institutional and disciplinary repository models for managing and exposing datasets. The real value will become apparent as Semantic technologies become established, at which stage the ever-increasing body of experimental data will provide new opportunities for knowledge discovery within and across disciplines.

7:00 PM Invited

The State of 3D Synthetic Microstructure Generation and Its Novel Applications: *Michael Groeber*[1]; Anthony Rollett[2]; Joseph Tucker[2]; Michael Jackson[3]; [1]AFRL; [2]Carnegie Mellon University; [3]BlueQuartz Software

The recent computational efforts to derive processing-microstructure and microstructure-property relationships have bolstered the need for digital representations of microstructure. To this end, synthetic microstructure generation serves as a viable and powerful path to providing microstructural volumes. This talk will present the state-of-the-art (SOA) in creating statistically-controlled microstructure instantiations that exhibit key, property controlling attributes such as: grain size, shape, texture, and neighborhoods. Additionally, this talk will illustrate a number of areas in which synthetic microstructure generation tools can aid in advancing the current SOA in a more rapid fashion than experimental data collection, which include, but are not limited to: 2D-to-3D extrapolation techniques, error and uncertainty quantification in data collection, statistical archival of microstructures, and microstructure design methodologies.

7:30 PM Question and Answer Period

7:45 PM

Model Reduction and Reconstruction of Realistic Microstructures for Computing Property Variability: *Nicholas Zabaras*[1]; Bin Wen[1]; [1]Materials Process Design and Control Laboratory

Due to the random nature of microstructures, property variability of a family of microstructures that share certain statistical constraints has become an interesting study area. However, microstructures are usually only known as a finite number of realizations, and the representation of a microstructure is high-dimensional. These facts prevent one from constructing the high-dimensional stochastic microstructure space and drawing samples directly from it. In this work, we propose a model reduction strategy to construct a low-dimensional surrogate space of random polycrystalline microstructures based on a set of given samples.

New samples are then generated from the surrogate space and mapped back to the original high-dimensional space. Variability of mechanical properties, e.g. stress-strain curve with error bars, of these microstructures can therefore be studied using collocation or Bayesian regression approaches by appropriate calling of an image-based physical solver.

8:05 PM
The OOF Project at NIST: *Stephen Langer*[1]; Andrew Reid[1]; Günay Dogan[2]; [1]National Institute of Standards and Technology; [2]NIST/Theiss Research

OOF, which stands for "Object-Oriented Finite elements", is an open-source materials modeling program being developed at NIST. Using OOF, users construct a finite element mesh based on a two or three dimensional micrograph of a real or simulated material. OOF can then perform virtual experiments on the mesh to determine microstructure/property relationships. OOF is designed to be easy to use by materials scientists and does not require a numerical analysis background. It can compute a wide variety of linear and nonlinear continuum physical phenomena, and can be easily extended. This talk will provide an overview of the OOF project and discuss its new 3D capabilities.

8:25 PM Break

8:45 PM
Fitting Laguerre Tessellations to the Microstructure of Cellular Materials: *Irene Vecchio*[1]; Katja Schladitz[1]; Claudia Redenbach[2]; [1]Fraunhofer ITWM; [2]University of Kaiserslautern

Cellular materials are employed in many fields, ranging from medical technologies to aerospace industry. In applications, understanding the influence of the microstructures on the physical properties of materials is of crucial importance. Stochastic models are a powerful tool to investigate this link. In particular, random Laguerre tessellations (weighted generalizations of the well-known Voronoi model) generated by systems of non-overlapping balls have proven to be a promising model for rigid foams. Model fitting is based on geometric characteristics estimated from micro-computed tomographic images of the microstructures. More precisely, the model is chosen to minimize a distance measure composed of several geometric characteristics of the typical cell. However, with this approach, inference of the model parameters is time consuming and needs manual interaction. In this talk, we investigate strategies leading to an automatic model fitting. Finally, this model fitting approach is applied to polymethacrylimide (PMI) foam samples.

9:05 PM
A Implicit Model for Generating Polycrtalline Structures and Unstructured Meshes: *LiangXing Lv*[1]; Liang Zhen[1]; Wenzhu Shao[1]; [1]Harbin Institute of Technology

A new method for the generation of three-dimensional model microstructures of polycrystalline materials is developed based on the Voronoi tessellation. The algorithm allows for the generation of grains with arbitrary aspect ratio and grain size distribution observed in different conditions. Besides the microstructure generator, a new algorithm for unstructured meshing of these polycrystalline aggregates was also developed. This algorithm is based on the physical analogy between a well organized unstructured mesh and a force equilibrated truss structure, and employed a specific grain boundary distance function d(r) and mesh size function h(r). The complex boundaries between grains are implicitly treated as internal interface by d(r)=0. In this manner, meshing of polycrystalline aggregates need not be executed in a bottom-up fashion, but directly based on the 3D connectives of nodes, and including the internal interfaces automatically. And mesh refinement near grain boundaries can be treated easily.

9:25 PM
Stereology and 3D Grain Boundary Network Analysis: *Bryan Reed*[1]; Brent Adams[2]; Joel Bernier[1]; Chris Hefferan[3]; Alisa Henrie[2]; Shiu Li[3]; Jonathan Lind[3]; Robert Suter[3]; Mukul Kumar[1]; [1]Lawrence Livermore National Laboratory; [2]Brigham Young University; [3]Carnegie Mellon University

We present experimental validation of a method for estimating 3D numerical grain boundary populations from measurements of individual cross sections. Such numerical populations are relevant to network topology and the modeling of intergranular failure modes in grain boundary engineered materials. We examine 3D reconstructions of stainless steel and copper generated by serial-section electron backscatter diffraction and high-energy x-ray diffraction microscopy. We show that 2D length fractions, 2D number fractions, and 3D number fractions are all distinct quantities when grain boundary type is correlated with grain boundary size. We also demonstrate that the last quantity may often be reliably inferred from the first two, eliminating the need to use 3D experimental methods to access at least some information about 3D network properties. Many of the twin boundaries are extremely complex, with highly reentrant shapes that can intersect a sample plane many times, giving a false impression of multiple separate boundaries.

3D Interfaces and Microstructural Evolution

Wednesday AM Room: Exhibit Hall
July 11, 2012 Location: Seven Springs Mountain Resort

8:15 AM Invited
Diffraction-based 3D Imaging of Microstructural Evolution: *Erik Lauridsen*[1]; [1]Risø-DTU

This talk review the current status of diffraction-based 3D imaging using synchrotron radiation, as well as addresses new developments in sub-micrometer non-destructive 3D diffraction-based imaging techniques. While conventional absorption contrast tomography remains an important tool for non-destructive 3D characterization, complementary diffraction-based 3D imaging techniques broaden the range of materials science problems which can be addressed using 3D X-ray imaging techniques. Examples on grain growth kinetics in metals and ceramics will be used to demonstrate the advantages of such techniques. Currently, the resolution of these diffraction-based imaging techniques is limited to the micron scale. However, many real materials have grain sizes in the range from a few hundreds of nanometers to a few microns and as such there is a strong scientific interest in extending the diffraction-based imaging techniques to higher resolution. Part of the talk will be devoted to new initiatives to bring diffraction-based imaging techniques into the sub-micron domain.

8:45 AM Invited
Interfacial Morphology and Evolution in Solid-Liquid Mixtures: J. Gibbs[1]; J. Fife[2]; *Peter Voorhees*[1]; [1]Northwestern University; [2]Swiss Light Source

We examine the evolution of solid-liquid mixtures during coarsening using insitu three-dimensional x-ray tomography. Due to the large data sets that are collected, automated segmentation of these images is essential. We have implemented forward projection algorithms that both remove artifacts and yield smooth interfaces in two-phase materials. Examples of this segmentation process will be given. Through this analysis we have determined the interfacial curvature, the local interfacial velocities, the correlation between interfacial curvature at a point and the average rate of change of interfacial area for interfacial patches with the same curvature. We find that, on average, the interfacial velocity is proportional to the mean curvature of the interface. Although such "motion by mean curvature" models have been proposed for systems involving short-range material transport, such as grain growth, they appear to hold in this system despite the long-range diffusional interactions among points on the interface.

9:15 AM Invited
3-dimensional Measurement and Description of the 5-parameter Grain and Phase Boundary Character in Steels: *Stefan Zaefferer*[1]; Peter Konijnenberg[1]; [1]Max-Planck-Institute for Iron Research

Interfaces in crystalline materials are characterized on a microscopic level by 5 parameters, the misorientation (3 parameters) and the interface normal vector (2 parameters). The physical properties of grain and phase boundaries depend more or less significantly on all of these parameters. It is therefore of high importance to quantify these parameters in order to understand details of microstructure formation and materials properties. FIB-EBSD tomography method is an effective and accurate tool for the determination of the 5D grain boundary character. The extraction of proper grain boundary information from the voxel (volume-pixel) based data sets obtained by FIB-EBSD requires procedures for alignment, boundary reconstruction and boundary smoothing. One new and powerful way is to describe each interface by an analytical function. We present our approach using a wavelet transform to fit the voxel data. This transform allows preservation and description of different levels of details of the boundaries.

9:45 AM Question and Answer Period

10:00 AM Break

3D Interfaces and Microstructural Evolution: Boundaries and Grain Growth

Wednesday AM	Room: Exhibit Hall
July 11, 2012	Location: Seven Springs Mountain Resort

10:15 AM
Quantitative Analysis of Three-dimensional Grain Growth: Trevor Keller[1]; *Dan Lewis*[1]; [1]Rensselaer Polytechnic Institute

Recent advances in computational techniques enable the efficient simulation of normal grain growth in three dimensions using the phase-field model. This opens the door to routine simulation of polycrystal systems with moderate numbers of grains on commodity computer hardware with reasonable simulation times. In this contribution, we analyze the evolution of distributions in grain size and topology as a function of increasing system size using multiorder parameters, such as multiphase field or quaternions. In addition, we apply Monte Carlo methods to investigate the sample space of triply-connected polyhedral graphs, which may be relevant to the grain growth analysis. Results of the simulations and statistical analysis of the data are discussed, with emphasis on implications for system size selection.

10:35 AM
The Shapes of a 3D Grain Growth Microstructure: *Emanuel Lazar*[1]; Jeremy Mason[2]; Robert MacPherson[1]; David Srolovitz[3]; [1]Institute for Advanced Study; [2]Lawrence Livermore National Laboratory; [3]Institute of High Performance Computing, A*Star

The most prevalent method of characterizing the topology of ideal grain-growth microstructures considers the distribution of faces as characterized by their number of sides, and of grains as characterized by their number of faces. This data is important but fails to tell the entire story. For example, of all twelve-faced grains what fraction are pentagonal dodecahedra? What fraction of grains have more than one triangular face or three hexagonal ones? Large front-tracking simulations developed by the authors and reported elsewhere have enabled us to begin answering these types of questions. We will briefly describe some graph-theoretic techniques we used to collect a more complete description of individual grains, and then report results from the authors' front-tracking simulations that have reached steady state with well over 250,000 grains.

10:55 AM
Topological Mechanism of Grain Growth: *Burton Patterson*[1]; Robert DeHoff[1]; Veena Tikare[2]; Zhiwei Sun[3]; David Rule[1]; Amy Adams[1]; [1]University of Florida; [2]Sandia National Laboratory; [3]University of Alabama at Birmingham

The topological model of grain growth describes the process in terms of the numbers of corners, edges and faces on grains and the topological events that change them. Topological analysis has been performed of microstructural evolution throughout grain growth using 3D Monte Carlo simulation, 3D x-ray analysis and conventional experiments. Growth paths of grain volumes and faces, topological contact affinities and distributions of grain volumes and faces have been determined. Integral mean curvature computed from 3DMC voxelated grain structures has been shown to compare well with that from serial section analyses. Volumetric growth rate was found to be linear with grain volume and integral mean face curvature. Affinity for contact between grain classes was modeled in terms of the product of the curvatures of the grain pairs forming boundaries. The combination of these related aspects of the topological model provide a comprehensive view of the topological nature of grain growth.

11:15 AM Break

11:30 AM
Distribution of Carbide Particles and Its Influence on Grain Growth of Ferrite in Fe-C Alloys Containing B and V: Takafumi Oikawa[1]; *Masato Enomoto*[1]; [1]Ibaraki University

The influence of pinning sites and spatial distribution of pinning particles on grain growth has been investigated theoretically and by computer simulation. In this study this problem is addressed experimentally; the number and size distribution of carbide particles in the matrix and at grain boundary sites, i.e. faces, edges and corners, were measured in Fe-0.1C-0.0005B and Fe-0.1C-0.09V alloys by serial sectioning. Grain corners were identified by recombination of grain boundaries and triangular annihilation. The proportion of particles at each grain boundary site was considerably greater than that of random distribution. The results were compared with modified Zener theories which assume that all grain boundaries are pinned by particles which give a f1/2 dependence of grain size (f is the volume fraction of particles), the Nishizawa et al's correlation model, and the Hunderi-Ryum's model which took the pinning at all grain boundary sites into consideration.

11:50 AM
Modeling Grain Boundary Interfaces in Pure Nickel: *Todd Turner*[1]; Jay Schuren[1]; Paul Shade[1]; Michael Groeber[1]; [1]Air Force Research Laboratory

This work presents two integrated modeling approaches to examine grain boundary interfaces in a Nickel-base superalloy utilizing a crystal plasticity based finite element model (CPFEM) coupled with high-energy x-ray diffraction experiments. The goal of this work is to validate modeling approaches through comparison to experimental data, and then use the models to gain insight into deformation at grain boundaries in superalloy polycrystals. The first study utilizes a bi-crystal tensile specimen and simulations to examine the effect of orientation on the development of localized plasticity or "hot-spots" near the boundary. Some orientation combinations exhibit localized plasticity along the boundary (bad-actor boundaries) while others do not. The second study embeds the bad actor grain boundary interfaces, as determined from the bi-crystal simulations, into a larger polycrystalline simulation utilizing the same CPFEM model framework to study deformation at these "characteristic" interfaces when subjected to the generalized loading conditions present in the polycrystalline microstructure.

12:10 PM
3D Stochastic Ginzburg-Landau Model of Non-Classical Nucleation: *Alexander Umantsev*[1]; [1]Fayetteville State University

The problem of incipience of a new phase—nucleation—is central for many branches of science including physics of crystallization of materials. Many properties of the nucleation scenario depend on the three dimensional structure of the critical nuclei. We consider a problem of homogeneous nucleation of a new phase in the framework of a stochastic Ginzburg-Landau model in three dimensions. We analyze dependence of the nucleation rate on the volume, driving force—the free energy difference between the old and new phases, and the intensity of fluctuations in the three-dimensional systems. Contrary to the traditional view, we find the nucleation rate to be inversely proportional to the square root of the volume instead of the volume itself. The critical nuclei in the model have large degree of ramification. The method allows us to study the structure and entire pre-nucleation path of the 'cluster' that leads to the critical precipitate of the new phase.

3D Interfaces and Microstructural Evolution: Structure and Morphology

Wednesday AM
July 11, 2012

Room: Sunburst
Location: Seven Springs Mountain Resort

10:15 AM
On the Three-dimensional Microstructure of Martensite in Carbon Steels: *Peter Hedström*[1]; Albin Stormvinter[1]; Annika Borgenstam[1]; Ali Gholinia[2]; Bartlomiej Winiarski[2]; Philip J. Withers[2]; Oskar Karlsson[3]; Joacim Hagström[3]; [1]KTH - Royal Institute of Technology; [2]University of Manchester; [3]Swerea KIMAB AB

The mechanical properties of high-performance steels are often reliant on the hard martensitic structure. It can either be the sole constituent e.g. in tool steels, or it can be part of a multi-phase structure as e.g. in dual-phase steels. It is well-known that the morphology of martensite changes from lath to plate martensite with increasing carbon content. The transition from lath to plate is however less known and in particular the three-dimensional (3D) aspects in the mixed lath and plate region require more work. Here the current view of the 3D microstructure of martensite in carbon steels is briefly reviewed and complemented by serial sectioning experiments using a focused ion beam scanning electron microscope (FIB-SEM). The large martensite units in the Fe-1.2 mass% C steel investigated here are found to have one dominant growth direction, less transverse growth and very limited thickening. There is also evident transformation twinning parallel to the transverse direction. It is concluded that more 3D analysis is required to understand the 3D microstructure of martensite in the mixed lath and plate region and to verify the recently proposed 3D phase field models of martensite in steels.

10:35 AM
Morphology and Crystallography of Annealing Twins in Austenite: *Milo Kral*[1]; Ben Gardiner[1]; [1]University of Canterbury

Annealing twins are a prominent feature in FCC metals with low stacking fault energy, such as austenitic steels. Previous work suggests that annealing twins have a significant effect on the physical properties of a material (e.g. yield strength and corrosion). The purpose of the current work was to determine the 3-dimensional morphology of annealing twins and the orientation/crystallography of their bounding surfaces. The task was accomplished by serial sectioning and EBSD mapping.

10:55 AM
Three-dimensional Morphology Due to Phase Separation in an Fe-Ni-Al Alloy Studied by STEM Tomography: *Syo Matsumura*[1]; Keisuke Ogata[1]; Satoshi Hata[1]; Minoru Doi[2]; Hideharu Nakashima[1]; [1]Kyushu University; [2]Aichi Insitute of Technology

HAADF-STEM tomography was applied to time-evolution of phase separation into (A2+B2) in an Fe-10.3 at%Ni-14.3 at %Al alloy. The alloy specimen was once annealed at 1173 K for one day to form ordered B2 precipitates in the disordered A2 matrix, and then was annealed at a lower temperature 973 K to promote further phase separation in both B2 precipitates and A2 matrix. With the progress of the second annealing at 973 K, spherical B2 precipitates are additionally formed in the A2 matrix and they grow according to the so-called 1/3 law. Phase separation takes place during the second annealing also within the B2 phase formed by the first annealing, resulting in a mottled morphology of (A2+B2). The 3-dimensional reconstructed images have characterized the mottled morphology as two-phase mixture about 70-80 nm periodicity along <100> directions.

11:15 AM Break

11:30 AM
3D Characterization of Microstructural Evolution in Anisotropic Ceramics: *Melanie Syha*[1]; Wolfgang Rheinheimer[1]; Michael Bäurer[1]; Wolfgang Ludwig[2]; Erik Lauridsen[3]; Daniel Weygand[1]; Peter Gumbsch[1]; [1]Karlsruhe Institute of Technology; [2]European Synchrotron Radiation Facility; [3]Risø National Laboratory

Microstructural evolution in strontium titanate has been investigated using X-ray Diffraction Contrast Tomography, a non-destructive technique allowing the simultaneous acquisition of morphologic and crystallographic information. Fully reconstructed microstructures of a cylindric specimen before and after an ex-situ heat treatment of 1h at 1600°C are presented alongside with detailed information on the crystallographic orientation of the grains forming the polycrystal. The quality of the reconstruction is critically analyzed by means of comparison to electron backscattering diffraction investigations with special emphasis on the accuracy of the grain boundary location and their orientation with respect to the crystallographic orientation of the adjacent grains. The results are discussed in the context of orientation dependent grain boundary properties and their influence on the morphology.

11:50 AM
Structural Evolution of Nanoporous Gold during Thermal Coarsening as Determined by X-ray Nano-tomography: Yu-chen Chen[1]; Steve Wang[2]; Yong Chu[3]; Wenjun Liu[2]; Ian McNulty[2]; Peter Voorhees[4]; *David Dunand*[4]; [1]Northwestern University, Argonne National Lab.; [2]Argonne National Lab.; [3]Brookhaven National Lab.; [4]Northwestern University

Nanoporous gold (np-Au) shows a bi-continuous nano-structure with pore and gold nano-ligament size as small as 5 nm. Np-Au has numerous potential applications including sensors, actuators, catalysts, super-capacitors and support structures for the electrodes of Li-ion. Thermal coarsening can be used to increase the feature size and tune the mechanical properties of np-Au. The 3D structural evolution of np-Au during coarsening was imaged by synchrotron x-ray nano-tomography. The size, curvature and surface normal orientation of gold nano-ligaments were characterized as a function of coarsening time (10 to 320 minutes) and temperature (550 to 650 ºC). The morphological anisotropy of np-Au was quantified by surface normal distribution and correlated to the preferred crystallographic orientation, as characterized by micro-beam Laue diffraction. This anisotropic coarsening behavior results in a non-self-similar evolution of the curvature distribution (scaled by feature size) of the features during coarsening.

12:10 PM

Exploring 3D Interfaces and Microstructural Evolution with Micro-Laue Diffraction: *Rozaliya Barabash*[1]; Jon Tischler[1]; John Budai[1]; Wenjun Liu[2]; [1]Oak Ridge National Laboratory; [2]Advanced Photon Source

Interfaces play a crucial role in the two-phase and multi-phase materials properties. Strain partitioning through the interfaces determines materials response to external fields. To understand the small-scale mechanical behavior and microstructural evolution in layered materials with submicron layer thickness, it is critical to have techniques to characterize the interface-adjacent defect distributions in 3D. Recently developed Polychromatic X-ray Microdiffraction (PXM) together with Differential Aperture X-ray Microscopy (DAXM) are used to characterize the 3D distribution of strain and dislocation density near buried interfaces in directionally-solidified layered Cr/NiAl composites after deformation by indentation. It is shown that composites' response to indentation is distinct from the single phase materials. Depth-dependent opposite sign strains are directly measured in individual Cr and NiAl submicron layers. Research supported by the Division of Materials Sciences and Engineering, U.S. Department of Energy. Data collection was carried out on beamline ID-34-E at the Advanced Photon Source.

Student Poster Session

Wednesday PM July 11, 2012 — Room: Exhibit Hall; Location: Seven Springs Mountain Resort

P3-01: 3D Visualisation of Crystallographic Pitting: *Alice Laferrere*[1]; Nick Parson[2]; Xiaorong Zhou[1]; George Thompson[1]; [1]The University of Manchester; [2]Rio Tinto Alcan

This research focused on understanding the mechanism of pitting corrosion in extruded Al-3XXX heat exchanger alloys. Conventional two dimensional examination of alloy surfaces and cross-sections was found insufficient to fully understand the 3 dimensional propagation of the corrosion front. In the present study, pits were studied with serial block-face scanning electron microscopy, a nanotomography technique using selective detection of backscattered electrons with serial in-situ sectioning by ultramicrotomy. The relationship between initiation and propagation of pitting and the microstructure and alloy composition was established. The investigation revealed that crystallographic pitting initiated within the alloy matrix and not the second-phase particles. Furthermore, the high resolution tomography provided direct evidence that link pit propagation to grain boundaries.

P3-02: 3D Analysis on the Effect of Creep Behavior on Phase Morphology of Duplex 2205 during the Continuous Annealing: *Heeyong Park*[1]; Bruno De Cooman[1]; [1]GIFT, POSTECH

High-temperature superplastic behavior brings about severe creep deformation during a continuous annealing of cold-rolled duplex stainless steels. In the present study, the effect of creep deformation triggered by the superplastic behavior on the microstructure of the 2205 duplex stainless steel during a continuous annealing was investigated by means of high temperature tensile test and 3D Robomat. Tensile tests were carried out in the different temperature range of 1000 and 1100^{o}C resulting in a high strain rate sensitivity of 0.67. The tensile samples deformed with different strain levels were used to investigate the effect of the creep deformation on the microstructure of the 2205 duplex stainless steel. A detailed three-dimensional optical microstructure was analyzed to reveal the influence of the superplastic deformation on the phase morphology.

P3-03: 3D Atom Probe Investigation of Nanoscale Austenite Reversion at Interfaces in a Martensitic Stainless Steel: *Lei Yuan*[1]; Dirk Ponge[1]; Dierk Raabe[1]; [1]Max-Planck-Institut fuer Eisenforschung

Austenite reversion during tempering of a Fe-13.6Cr-0.44C (wt.%) martensite results in an ultra-high strength martensitic stainless steel with excellent ductility. The austenite reversion mechanism is coupled to the kinetic freezing of carbon during partitioning at the interfaces between martensite and retained austenite and to carbon segregation at martensite-martensite grain boundaries. The reverted austenite acts as a barrier to prevent cracks development during deformation. The austenite reversion process, nano-carbide precipitation, and carbon segregation have been characterized by atom probe tomography (APT) in order to develop the structure-property relationships that control the material's strength and ductility. A 3D reconstruction was established base on the APT results especially at the interfaces.

P3-04: 3D Microstructure Analysis in Macro-micro Scale: *Yeom Kyu Jung*[1]; Seong Bum Son[1]; Chan Soon Kang[1]; Jong Soo Cho[1]; Jeong Tak Moon[2]; Heung Nam Han[1]; Kyu Hwan Oh[1]; [1]Seoul National University; [2]MK Electron

Three dimensional microstructure data enables us to realize actual size, shape of feature and feature connectivity. However 2D measurement of mean feature size and shape distribution is inaccurate compared to 3D analysis. The purpose of this study is to understand topological property and characterization in 3D microstructure at different length scale such as macro-micro scale. We utilize optical microscopy and focused ion beam (FIB) for image acquisition through serial sectioning method. Fiducial mark with using Vickers indenter is adopted to align images and measure the depth of slices at macro scale. Serial sectioning method through the FIB could attain 3-dimensional volumetric information in micro scale. The work demonstrates that 3D analysis technique for macro-micro scale provides microstructure information that cannot be visualized with using typical 2D analysis.

P3-05: 3D Microstructure Construction of Sintered ZrO2 under Different Sintering Conditions: *Zhenbo Xia*[1]; Kathy Lu[1]; [1]Virginia Polytechnic Institute and State University

Sintering of nanoparticle materials requires much greater control over particle packing homogeneity and nano-/micro-structural evolution. Currently, there is a lack of quantitative description and evaluation of nano-/micro-structural evolution during sintering. This has impeded decoupling of different sintering mechanisms and quantification of the relative contribution of these mechanisms to sintering densification and kinetics. In this study, the microstructure evolution of yttria stabilized ZrO2 after different sintering conditions is presented. Focus ion beam (FIB) is used as a critical tool for sintering microstructure evolution understanding. 3D images are constructed with Amira software based on a series of 2D images obtained from FIB by cutting the samples slice-by-slice successively with an interval of 10 nm. Pore volume fraction and size distribution, as well as grain-pore interfacial areas of the sintered samples are calculated by IDL software using the 3D images. The results are discussed from both theoretical and experimental points of view.

P3-06: 3D Microstructures of Sb_2Te_3 Precipitates in PbTe Matrix and Their Elongations with Prediction by a Weak Compatibility Condition: *Xian Chen*[1]; Shanshan Cao[2]; Teruyuki Ikeda[3]; Jeffrey Snyder[4]; Dominique Schryvers[5]; Richard James[1]; [1]University of Minnesota; [2]South China University of Technology; [3]PRESTO; [4]California Institute of Technology; [5]University of Antwerp

We propose that a weak compatibility condition predicts the elongated directions for Widmanstatten type precipitates. The distribution of the elongated directions of precipitates lies on a family of crystallographically equivalent cones in 3D determined by a certain transformation strain matrix obtained independently. A 3D visualization and digitization method is developed to show how the cone variants control the preferred growth directions during precipitation of Sb2Te3 in PbTe matrix. A series of two-dimensional secondary electron images are acquired along the direction perpendicular to the imaging plane. By pixelating all the images and calculating the position vectors on the surface of each precipitate, the elongation directions are calculated using a 3-dimensional ellipsoidal fitting for 182 precipitates. The 3D plot of the elongation directions shows that their spacial orientations are close to four predicted cones with a standard deviation of 5.6°. The length along the elongation directions reveals an asymmetric distribution with a mean value of about 240 nm.The total volume fraction of the precipitates is 8.3 % and the average area of the precipitates per volume is 0.68 µ m(-1) by one point statistical calculation. These results build on a study presented previously by analyzing a significantly bigger data set and by including the length distribution and 1-point statistics.

P3-07: Bulk Three-dimensional Magnetic Domain Structure in a Slightly Misoriented (110)[001] FeSi Single Crystal: Sunmi Shin[1]; Rudolf Schaefer[2]; *B. C. De Cooman*[1]; [1]Pohang University of Science and Technology; [2]IFW Dresden

Grain-oriented (GO) silicon steel is used in the core materials for power transformers requiring high permeability and low losses. The predominant {110}<001> orientation of the steel meets the stringent loss requirements for the application due to the development of the sharp texture. For the further reduction of loss, the control of the magnetic domain structure is indispensable. At a 3~7° misorientation, which is the typical misorientation for GO steel, a supplementary domain structure appears. The creation and annihilation of 90° domain walls in this structure are believed to increase the losses. The internal domain structure, however, has never been observed. Here, we imaged the 3D magnetic domain structure of a 3~6° misoriented (110) Fe-6.6%Si steel by using Libovický's method and serial sectioning. The 3D domain structure was reconstructed using the serial images for a solid volume of 1700×422×800 μm^3. The observed structure differ from the models predicted by domain theory.

P3-08: Calculation of Grain Boundary Character Distribution from Three Dimensional EBSD Data: *Hadi Pirgazi*[1]; Roumen Petrov[2]; Leo Kestens[1]; [1]Gent University; [2]Delft University of Technology

It is well known that from 3D EBSD data more additional microstructural information can be obtained, particularly with regards to microtexture and grain boundary character distribution (GBCD). To observe the grain boundary character distribution (GBCD) in different metals, numerous experimental 3D EBSD data sets were collected employing the manual serial sectioning technique. The thickness of each layer was approximately 10% of the average grain size and the number of sections varied from 8 to 12 depending on the material. An alignment algorithm based on minimum misorientation was applied together with a triangulation algorithm to reconstruct the 3D microstructure. The distribution of GB plane normals was derived and represented in an inverse pole figure projection. The orientation of GB plane normals with respect to the crystal orientation of adjacent grains was evaluated and discussed in terms of the local GB energy, for different materials with different crystal structures.

P3-09: Deformation Mechanisms Studied in Commercially Pure Titanium by Combined use of X-ray Diffraction Contrast Tomography (DCT) and Scanning Micro-diffraction Procedures: *Laura Nervo*[1]; Michael Preuss[2]; João Quinta da Fonseca[2]; Wolfgang Ludwig[3]; Andrew King[4]; [1]ESRF & University of Manchester; [2]University of Manchester; [3]INSA de Lyon; [4]ESRF

The combination of the diffraction contrast tomography with the line beam and pencil beam scanning procedures offers new possibilities for 3D in-situ observation of deformation and damage mechanisms in the bulk of polycrystalline materials. The X-ray DCT is a variant of the 3D X-ray diffraction (3DXRD) microscopy technique enabling simultaneous reconstruction of the 3D microstructure (shape and orientation) in suitable polycrystalline materials, along with the absorption map of the specimen. The x-ray diffraction contrast tomography (DCT) methodology provides access to the 3D shape, orientation and elastic strain state of the individual grains from polycrystalline sample volumes containing up to thousand grains. DCT is used in the present study to investigate the twinning mechanism operational during plastic deformation of polycrystalline commercially pure Titanium (hcp). Twinning is an important deformation mode in metals with a hexagonal close-packed (hcp) crystal structure because of the limited number of easy slip modes. During twinning atom moves only by a small distance but in a co-operative process resulting in an overall crystal rotation of the twinned volume. To date, our understanding of twin nucleation criteria and twin growth is very limited, which makes a physical meaningful implementation of twinning in crystal plasticity models difficult. In the present study, a commercially pure titanium sample was compressed to different levels of plastic strain while undertaking DCT scans. The aim of the in-situ experiment was to study the evolution of twins in relation to plastic strain and grain neighbourhood as well as identifying the grains that deform by slip first. The data from the DCT experiment will be compared with a finite element crystal plasticity model that will also provide information about the stress state of individual grains.

P3-10: Design of Virtual 3D Micostructures with Controlled Grain Size and Orientation Distribution: *Edgar de Araujo*[1]; K. Verbeken[1]; L.A.I. Kestens[1]; [1]Gent University

For a wide variety of model calculations a 3D microstructure is required as input. Although experimental data are frequently used to this purpose, 3D microstructures are difficult to measure experimentally. In order to circumvent these difficulties, a virtual microstructure generator is developed to reproduce a specific 3D material microstructure with various specific features of a real microstructure whilst matching the boundary conditions imposed by a number of distribution functions. In the current paper a new method for generating 3D microstructures is proposed. The method allows designing an assembly of contiguous grains with control of various distributions pertaining to topological features such as grain size, grain shape and number of neighbors. Our method uses a sequential polydisperse sphere packing algorithm that employs molecular dynamics and Laguerre diagram algorithms to generate contiguous microstructures in continuous space.

P3-11: Four-dimensional Characterization of Coarsening of Complex Microstructures via Phase-field Method: *Chal-Lan Park*[1]; Peter W. Voorhees[2]; Katsuyo Thornton[1]; [1]University of Michigan; [2]Northwestern University

Coarsening is an important material phenomenon that can impact material properties. While coarsening of spherical precipitates has been well studied, the understanding of the evolution of complex microstructures during coarsening is still incomplete. We use the phase-field method to simulate coarsening of bicontinous structures. Using the results, we calculate interfacial properties such as curvature, and their time derivatives, to elucidate the dynamics of coarsening for complex morphologies. These quantities are then mapped to distribution plots to understand the correlation between the local properties and their rates of change. Specifically, the time derivative of the interfacial mean curvature can quantify the morphological evolution of the complex microstructure undergoing coarsening. We also propose that the complex microstructures of symmetric mixtures can be described in terms of one of the principal curvatures, which is analogous to the radius of precipitates for microstructures consisting of spherical precipitates.

P3-12: In-situ Characterization of Entrainment Defects in Liquid Al-Si-Mg Alloy: *Yang Yue*[1]; William Griffiths[1]; Julie Fife[2]; Nick Green[1]; [1]University of Birmingham, UK; [2]Swiss Light Source, PSI

Entrainment defects occur frequently in aluminium alloy castings during the mould-filling process, and are very detrimental to both mechanical properties and reliabilities. The formation mechanisms and influences of these defects have been discussed previously, but the behaviour of the defects in liquid metal and their evolution during solidification have not been studied in detail. In this research, samples of Al-Si-Mg alloy A356 that contained entrainment defects were scanned using ultra-fast synchrotron X-ray radiography at the Paul Scherrer Institute, using their TOMCAT beamline. The defects were directly viewed at both room temperature, and in a fully liquid state. The reconstructed images showed three different pore morphologies, namely, entrained pores, tangled double oxide films and closed cracks. The evolution of the morphology of the entrainment defects was studied, which gave direct evidence of the mechanism of morphological changes of the defects, and the relationship between entrainment defects and microporosity.

P3-13: Influence of Serial Section Thickness on the Measurement Precision of 3D Grain Volume and Surface: *Binbin Zhang*[1]; Guoquan Liu[1]; [1]USTB

To seek for the balance between the efficiency and accuracy of three-dimensional (3D) quantitative characterization on grain structures, the selection of the section thickness in serial sectioning technique is of great importance. Taking the grain structures generated by Potts model Monte Carlo simulation as the study object, this paper investigates the influence of serial section thickness on the measurement of grain volume and grain surface area. The results indicate that the values of h/l should be less than 0.123 and 0.188 for the measurement of grain volume and grain surface area respectively, in order to insure that the relative error of the measurement is less than 5% and 10%, where h is the section thickness and l is the average grain intercept. The results provide the section thickness selecting rules in the serial sectioning method, which is helpful for the quantitative characterization study of polycrystalline microstructures.

P3-14: Investigation of Creep Damage in Martensitic 9-12% Cr Steel using Synchrotron X-ray Micro-tomography: *Christian Schlacher*[1]; Peter Mayr[2]; Francisca Mendez Martin[3]; Chiradeep Gupta[4]; Hiroyuki Toda[4]; Kentaro Uesugi[5]; Yoshio Suzuki[5]; Christof Sommitsch[3]; [1]Graz University of Technology ; [2]Chemnitz University of Technology; [3]Graz University of Technology; [4]Toyohashi University of Technology; [5]Japan Synchrotron Radiation Research Institute

Creep resistant martensitic 9-12% chromium steels are key materials for the construction of highly efficient steam power plants. During long-term high temperature service in the regime of creep, a drop of strength caused by microstructural degradation and formation of localized damage was observed. The formation of creep voids and their combination to micro- and macro-cracks has been identified as the main reason for these early failures. In this work, creep tests at 650°C have been carried out for 9-12% Cr steels up to 24.000 hours at different stress levels. The creep strength was analyzed and the evolution of damage was investigated using synchrotron micro-tomography supported by electron microscopy. By synchrotron micro-tomography, the 3-dimensional void distribution was visualized for different creep loads corresponding to different time-to-ruptures. The correlation of long-term creep testing data and a 3D damage mapping allows a completely new view on the basic failure mechanism at elevated temperatures.

P3-15: Microstructure-based Life Modeling of Ni-based Superalloys: *Joseph Tucker*[1]; Albert Cerrone[2]; Anthony Rollett[1]; Anthony Ingraffea[2]; [1]Carnegie Mellon University; [2]Cornell University

Integrating computational materials science into materials design techniques that traditionally rely on experimentation has the potential to drastically reduce the deployment time of advanced materials to market. One such opportunity is modeling fatigue phenomena of Ni-based superalloys used in aircraft turbine engines. By producing high fidelity microstructural representations of these material systems, accurate response is evoked in physics-based models. If the environment of the weakest link is present in these synthetic microstructures, strain localizations will evolve at these locations. These microstructural features can then be identified and designed against to improve the next generation of materials.

P3-16: Microstructure Change of SOFC Anode during Long Term Operation using 3D Reconstruction: *Harshil Parikh*[1]; Arthur Heuer[1]; Mark De Guire[1]; Zhien Liu[2]; Richard Goettler[2]; [1]Case Western Reserve University; [2]Rolls-Royce Fuel Cell Systems (US) Inc.

Changes in the microstructure of a Ni-YSZ based anode in a Solid Oxide Fuel Cell (SOFC) stack has been studied using 3D reconstruction. The SOFC was operated at 925 °C for 8500 hours as part of an evaluation of the long term performance of such SOFCs. Notable changes in the microstructure of the anode was observed, and the 3D reconstruction technique was crucial in understanding how the microstructure evolved with time. The three phases of the SOFC anode – the metallic electronic conductor, the ceramic ionic conductor, and the pore phase crucial to the density of the three phase boundaries -- were characterized using key structural parameters such as volume fraction of each phase, particle diameters, tortuosity and surface area.

P3-17: Modeling 3D Grain Coarsening Based on Tomography Data: *Melanie Syha*[1]; Daniel Weygand[1]; Peter Gumbsch[2]; [1]Karlsruhe Institute for Technology; [2]Karlsruhe Institute of Technology

The experimental 3D characterization of the morphology and crystallography of anisotropic ceramics using X-ray Diffraction Contrast Tomography implies ample opportunities to improve the modeling of these materials. 3D reconstructions of cylindric strontium titanate microstructures have been imported to a 3D mesoscale grain coarsening model which is able to handle misorientation and inclination dependent grain boundary properties. The evolution of these structures has been simulated using systematically varied grain boundary properties and the simulated structures were compared to reconstructions of the input structures after they have seen an ex-situ heat treatment of 1h at 1600°C. This approach presents a unique way to validate the grain coarsening model and to establish a grain boundary property database for the modeling of microstructure evolution in strontium titanate. The results are critically discussed in terms of choice of parameters and applicability to other materials.

P3-18: Novel 3D Characterization for the Advanced Understanding of Stereological Quantification of a+ß Titanium Alloys: *John Sosa*[1]; Daniel Huber[1]; Vikas Dixit[1]; Peter Collins[2]; Hamish Fraser[1]; [1]The Ohio State University; [2]University of North Texas

Advanced three-dimensional data collection techniques such as RoboMet-3D™ and DualBeam™ FIB/SEM has led to rapid acquisition of robust datasets across length scales. This work addresses the collection, processing, and analysis of datasets containing microstructural features such as equiaxed-a and a-laths in a+ß titanium alloys. In regard to equiaxed-a, rigorous dataset collection, along with innovative 3D feature-find and separation algorithms have allowed for robust three-dimensional quantification. Comparing such quantification with its stereological complement has improved the understanding of stereological metrics and their role in neural network property-predictive models. With regard to a-laths, novel 3D quantification algorithms have permitted extensive characterization of their complex morphology. Additionally, powerful two-point correlation image segmentation has permitted the unique colony-by-colony analysis of 2D and 3D microstructures and has provided valuable insight into the stereological requisites of a-lath quantification.

P3-19: Pitfalls in Direct 3D Characterization for Microstructural Quantification of a+ß Titanium Alloys: *Daniel Huber*[1]; John Sosa[1]; Margaret Noble[1]; Vikas Dixit[1]; Peter Collins[2]; Hamish Fraser[1]; [1]The Ohio

State University; [2]University of North Texas

Robust and sophisticated methods of characterization have been used to develop neural networks that provide an interpolative prediction of the interrelationship between microstructure and properties. The accuracy of the output of such models depends on both the accuracy and fidelity of the methods of characterization, and the variance and distribution of the input data. This work focuses on three tasks: firstly, a comparison of direct 3D to 2D methods of characterization; secondly, the measured variance and distribution of quantified microstructural features in a+ß processed Ti-6Al-4V; and thirdly, determination of the "Representative Volume Element". The results of these three investigations will be described. Although direct 3D methods of characterization are inherently more accurate than conventional 2D procedures, the pitfalls associated with this high fidelity approach will be discussed. This research has been supported in part by the US ONR.

P3-20: Quantifying the Effect of Spatial Resolution on the Accuracy of 3D Feature Characterization: *Gregory Loughnane*[1]; Ramana Grandhi[1]; Raghavan Srinivasan[1]; Michael Uchic[2]; Michael Groeber[2]; Matthew Riley[3]; Megna Shah[4]; [1]Wright State University; [2]Air Force Research Laboratory; [3]University of Idaho; [4]UES, Inc.

The choice of spatial resolution for experimentally-collected serial sectioning data is often based on general rules of thumb with regards to the minimum number of sections required to interrogate the features-of-interest. This work aims to quantitatively determine the minimum number of sections relative to the mean feature size to achieve a user-defined accuracy for selected attributes such as the grain size distribution, for both the mean value as well as for the full distribution. State-of-the-art 3D materials analysis software, DREAM.3D, is used to generate synthetic (digital) microstructural volumes from user-supplied statistical input distributions. The uncertainty in selected characterization attributes as a function of spatial resolution is quantified via virtual down-sampling of the digital microstructure; in particular by comparing measurements made on the down-sampled volumes to those obtained from the original reference volume.

P3-21: Quantitative Analysis and Comparison of γ' Precipitate Shapes in a Series of Ni-based Superalloys: *Patrick Callahan*[1]; Marc De Graef[1]; [1]Carnegie Mellon University

The shapes of secondary γ' precipitates in a series of Ni-based superalloys were determined by FIB serial sectioning. The alloys, designated UM-F, belong to a series of alloys with compositional differences and, hence, different lattice misfits and precipitate shapes. The precipitate shapes were analyzed quantitatively by means of second order 3D moment invariants and their distributions were compared using the Hellinger distance. Moment invariants are non-linear combinations of moments that are invariant to classes of coordinate transformations. They have been used extensively in computer vision, and, more recently, to quantitatively analyze shape in materials science. The contribution will briefly describe moment invariants and how they can be used to describe shapes; moment invariant distributions of the precipitate shapes from several samples of the UM-F series alloys will be compared. We will conclude the presentation with a short discussion of the effect of sampling resolution on the quantitative description of shape.

P3-22: Reconstruction of γ' Precipitate Shapes in Ni-base Superalloys by Means of 3D Zernike Functions: *Patrick Callahan*[1]; Marc De Graef[1]; [1]Carnegie Mellon University

The secondary γ' precipitate shapes in two Ni-based superalloys, one from a UM-F20 alloy with cuboidal precipitates, and one from a René-88 alloy with more complex dendritic precipitates, have been decomposed and reconstructed using 3D Zernike functions, which are orthogonal over the unit ball; they can be used to decompose an arbitrary shape scaled to fit inside an embedding sphere into spherical harmonics. Relatively complex shapes can be decomposed into, and reconstructed from, 3D Zernike functions. In this talk, we will start by introducing the 3D Zernike functions and a method for deriving expressions for Zernike moments from the more familiar geometric moments. Examples of 3D Zernike functions and moments for more general shapes of a sphere, an ellipsoid, and a cube will be given; then, the reconstructions of precipitates from the two Ni-base superalloys will be discussed.

P3-23: Representation in 3D and Stress Response of Tin Whiskers: *Benjamin Anglin*[1]; Pylin Sarobol[2]; Aaron Pedigo[2]; Wei-Hsun Chen[2]; Ricardo Lebensohn[3]; John Blendell[2]; Carol Handwerker[2]; Anthony Rollett[1]; [1]Carnegie Mellon University; [2]Purdue University; [3]Los Alamos National Laboratory

Whisker growth is a well-known stress relief mechanism in thin films and is commonly found in tin finishes for electronic component applications. With the push towards reduction of lead in commercial use, tin and lead-free tin alloys have become ubiquitous replacements for lead-tin solders. However, whiskers can bridge interconnects and cause short-circuit failure. It is generally known that stresses in the finishes arise from intermetallic compound growth, thermal expansion anisotropy of β-tin and thermal expansion mismatch of the finish and leadframe. An FFT method for simulating eigenstrains will be used to compute the mechanical response of a measured microstructure of a tin finish with a leadframe. Whiskers typically form at grain boundaries but do not penetrate the entire depth of the finish. The depth and representation of the whisker grain will be varied and dependence on the accumulation of stresses will be presented, as well as the grain neighborhood.

P3-24: SEM-based Electron Tomography of Turfs Comprised of Lineal Structures: *Osama Fakron*[1]; D.P. Field[1]; [1]WSU

In recent years, electron tomography (reconstruction of three-dimensional information from a tilt series of bright field images obtained in the TEM) has attracted the attention of electron microscopists and materials researchers. In this research the electron tomography technique has been extended to imaging loosely intertwined lineal structures imaged by secondary electron imaging in the SEM. The expected application is to investigate the structure of carbon nanotube turfs before and after deformation. For imaging, the specimen was tilted from -10 to 60° by one degree steps. Three dimensional images were reconstructed for a test sample of fine steel fibers by EM3D 2.0 electron tomography software. Chimera visualizing software used in visualizing the created three dimensional images, getting (X, Y, Z) position, and calculating the tortuosity.

P3-25: The Microstructure of RR1000 Nickel-base Superalloy: The FIB-SEM Dual-beam Approach: *Stephen Croxall*[1]; Mark Hardy[2]; Howard Stone[1]; Paul Midgley[1]; [1]University of Cambridge; [2]Rolls Royce plc

Nickel-base superalloys are aerospace materials that exhibit exceptional mechanical properties and corrosion resistance at very high temperatures. R1000 is used in discs in gas turbine engines, where temperatures reach in excess of 650°C with high mechanical stresses. Study of the microstructure at the micron and sub-micron level has conventionally been undertaken using scanning electron microscope images, meaning the underlying 3D microstructure can be inferred only with additional knowledge. Using a dual-beam workstation, we are able to interrogate directly the 3D microstructure using a serial sectioning approach. The 3D data set, typically 750μm^3 , reveals microstructural detail with lateral resolution of 8.3nm and a depth resolution dictated by the slice thickness, typically 50nm. Morphological and volumetric analysis of the 3D reconstruction of RR1000 superalloy reveal analysis of the microstructure hitherto unseen. The authors would like to acknowledge the EPSRC, University of Cambridgeand Rolls-Royce plc for financial support.

P3-26: The Time Evolution of Three Grains in a Thin Film: *Vadim Derkach*[1]; Amy Novick-Cohen[1]; Arcady Vilenkin[2]; [1]Technion-IIT; [2]Hebrew University

We consider of a thin film containing three grains and follow their evolution numerically. Within this configuration, the three grains are separated by grain boundaries which evolve by motion by mean curvature, and the grain boundaries intersect the exterior of the thin film. The exterior surface is assumed to evolve by surface diffusion, thermal grooving occurs along the triple junction lines where the grain boundaries intersect the exterior surface, and the quadruple junction which forms where the thermal grooves intersect deeps as a function of time. Isotropy is assumed, and the motion is followed numerically using an implicit time scheme, finite difference approximations, and a staggered spatial grid. The simultaneous deepening of the thermal grooves, the quadruple junction, and the corner points is studied, and all are found to roughly follow a t^{1/4} law. Details will be reported.

P3-27: Three-dimensional Atomic and Defect Structures of Ultra Thin Au and Au-alloy Nanowires: *Chun-Hsien Wu*[1]; Niven Monsegue[1]; William Reynolds[1]; Deborah Aruguete[2]; Michael Hochella[1]; Xin Jin[1]; Ge Wang[1]; Mitsuhiro Murayama[1]; [1]Virginia Tech; [2]National Science Foundation

Electron tomography and high-resolution transmission electron microscopy techniques were used to investigate the formation mechanism of colloidal synthesized <111> oriented ultrathin gold and gold-alloy nanowires with diameters less than 10nm.Nanowires fabricated by colloidal synthesis methods can have multiple growth directions, and the atomic structure and functional properties of those nanowires are strongly influenced by the growth direction. Both pure metal (e.g. Au, Ag) and metal compounds (e.g. GaP, InP) nanowires with a <111> growth direction tend to have a fine, high density twinned structure, that leads to high strength, high electrical conductivity with high break down current so they have potential applications in electronic devices. We observed surface/internal defect structures with atomic resolution electron tomography. We discuss the relationship of the three-dimensional morphology, defect structure, and growth orientation of the nanowires in terms of the defect structure of the wires and surface energy calculations.

P3-28: Three-dimensional Investigation of Void Growth Leading to Fracture in Commercially Pure Titanium: *Marina Pushkareva*[1]; Jérôme Adrien[2]; Eric Maire[2]; Arnaud Weck[1]; [1]University of Ottawa; [2]INSA de Lyon

The fracture process of commercially pure titanium was visualized in model materials containing artificial holes. These model materials were fabricated using a femtosecond laser coupled with a diffusion bonding technique to obtain voids in the interior of titanium samples. Changes in voids dimensions during in-situ straining were recorded in three dimensions using x-ray computed tomography. Void growth and coalescence obtained experimentally were compared with analytical models. In some cases, the models predicted well void growth and coalescence while in other cases, predictions were very poor. This was justified in terms of grain orientation. Depending on the number of grains between voids and the grains orientation, two types of fracture behaviors were observed: i) brittle fracture when grains were in a hard orientation and when few grains were present between voids; ii) ductile fracture when grains were in a soft orientation and when several grains were present between voids.

P3-29: Three Dimensional Simulation of Dendritic Solidification by Lattice Boltzmann and Cellular Automaton Methods: *Mohsen Eshraghi*[1]; Sergio Felicelli[1]; [1]Mississippi State University

A three-dimensional (3D) numerical model was developed to simulate the dendritic microstructure during solidification of binary alloys. Lattice Boltzmann method was used to simulate the transport phenomenon and a cellular automaton algorithm was employed to capture the solid/liquid interface. A weighted mean curvature approach was used to incorporate the surface energy and anisotropy effects in three dimensions. The model successfully reproduced the morphology of the 3D dendrite with well-developed side branches. Considering the high computational demands of 3D simulations and special characteristics of lattice Boltzmann and cellular automaton methods, like inherent parallel structure, the proposed model can be considered as an efficient tool for prediction of dendritic microstructure during solidification of alloys.

P3-30: Subgrain Boundary Identification in 3D EBSD Data through Fast Multiscale Clustering: *Brian Soe*[1]; Cullen McMahon[1]; David Golay[1]; Zakaria Quadir[2]; Michael Ferry[2]; Lori Bassman[1]; [1]Harvey Mudd College; [2]University of New South Wales

Complete and accurate characterization of subgrain microstructural features permits study of the relationships among loading, microstructure and properties in plastically deformed metals. 3D electron backscatter diffraction (EBSD) data can produce reconstructed crystallographic volumes, however low-angle subgrain boundaries cannot be determined simply with point-to-point misorientation thresholding because many are gradual transitions in orientation. We demonstrate a novel 3D implementation of the data segmentation technique Fast Multiscale Clustering, which uses a quaternion representation of orientation and a corresponding distance metric. Examples of the morphological analysis that can be obtained from the results will be presented, from the 3D segmentation of microbands in die-compressed nickel single crystal and uniaxially loaded commercially pure aluminum.

P3-31: Use of Serial Sectioning to Characterize Local Grain Boundary Structures in Nickel-Based Superalloys: *Jennifer L.W. Carter*, John M. Sosa1, Paul A. Shade[2], Hamish L. Fraser[1], Michael D. Uchic[2], Michael J. Mills[1] ; [1] Department of Materials Science and Engineering, The Ohio State University; [2] Air Force Research Laboratory, Materials & Manufacturing Directorate, AFRL/RXLM, Wright Patterson AFB

Full field strain mapping experiments on a polycrystalline Ni-based superalloy have shown a variety of grain boundary behavior based on surface features, including grain boundary sliding (GBS) and strain localization. Transmission electron microscopy (TEM) work has indicated that boundaries showing these different deformation behaviors may have unique subsurface topography. In this study, serial sectioning via focused ion beam milling was used to gain further insight into the 3D grain boundary network of two grain boundaries: one that experienced grain boundary sliding and another that experienced strain accumulation. Consistent with the TEM analysis, the serial sectioning has indicated that the subsurface grain boundary topography are distinctly different: the GBS boundary is relatively planar and simple in nature, while the grain boundary experiencing strain accumulation has a complex network of subsurface grain boundaries. Full field strain mapping experiments on a polycrystalline Ni-based superalloy have shown a variety of grain boundary behavior based on surface features, including grain boundary sliding (GBS) and strain localization. Transmission electron microscopy (TEM) work has indicated that boundaries showing these different deformation behaviors may have unique subsurface topography. In this study, serial sectioning via focused ion beam milling was used to gain further insight into the 3D grain boundary network of two grain boundaries: one that experienced grain boundary sliding and another that experienced strain accumulation. Consistent with the TEM analysis, the serial sectioning has indicated that the subsurface grain boundary topography are distinctly different: the GBS boundary is relatively planar and simple in nature, while the grain boundary experiencing strain accumulation has a complex network of subsurface grain boundaries.

Applications of 3D Experimental Techniques Across Length Scales: Non-Destructive Techniques

Wednesday PM Room: Exhibit Hall
July 11, 2012 Location: Seven Springs Mountain Resort

6:30 PM Invited
Ultra Fast Tomography: New Developments for 4D Studies in Material Science: *Pierre Lhuissier*[1]; Mario Scheel[2]; Marco Di Michiel[2]; Elodie Boller[2]; Jérôme Adrien[3]; Eric Maire[3]; Luc Salvo[1]; Jean-Jacques Blandin[1]; Michel Suery[1]; [1]SIMaP/GPM2-CNRS-Grenoble University; [2]ESRF; [3]MATEIS - INSA Lyon

X-ray tomography has become a widely used 3D characterization technique in materials science using either laboratory tomographs or large X-ray facilities. The two main improvements in the last decade are the decrease of the spatial resolution down to tens of nanometers and also the decrease in acquisition time of a complete scan down to 1 second with 2 µm spatial resolution. The aim of this presentation is to focus on the second point. We will present the technical problems arising due to ultra fast acquisition (development of specific sample environment) and its application in material science. We will show, that thanks to ultra fast tomography, it is now possible to investigate material science problems in 4D (crack propagation in metals and high temperature deformation).

7:00 PM Invited
High Energy X-ray Diffraction Microscopy Microstructure Mapping: *Robert Suter*[1]; Shiu Fai Li[2]; Christopher Hefferan[1]; Jonathan Lind[1]; Reeju Pokharel[1]; Ulrich Lienert[3]; Anthony Rollett[1]; [1]Carnegie Mellon University; [2]Lawrence Livermore National Laboratory; [3]Argonne National Laboratory

High energy diffraction microscopy (HEDM) is a suite of x-ray measurements implemented at Argonne National Laboratory's Advanced Photon Source. The measurements characterize crystallographic properties of individual grains deep inside of polycrystalline materials. Here, we discuss orientation mapping measurements that are a three dimensional and non-destructive analog of electron backscattering diffraction (EBSD) based orientation imaging at surfaces. The measurements use a line focused beam with energies $geq 50$ keV to image diffraction peaks from planar sections of millimeter dimensioned samples. A forward modeling method is used to reconstruct spatially resolved crystal orientations with $approx 1 mu$m spatial and 0.1 degree orientation resolution. High performance computations reconstruct volumes of the order of a cubic millimeter in both well ordered and defected materials. Methods continue to be developed to extract detailed characterizations of structure and evolution and to make direct comparisons to computational models. Several case studies will be described and presented in other talks.

7:30 PM Question and Answer Period

7:45 PM
High-speed Micro Imaging with Polychromatic Hard X-ray Synchrotron Radiation for Academic and Industrial Applications: *Elodie Boller*[1]; Paul Tafforeau[1]; Alexander Rack[1]; Carmen Soriano[1]; Sophie Sanchez[1]; [1]ESRF

Synchrotron-based hard X-ray microtomography (micro-CT) is a non-destructive imaging technique, which allows obtaining three-dimensional images of bulk samples with up to sub micrometer spatial resolution. High resolution micro-CT instruments were developed at the European Synchrotron Radiation Facility, and in particular at the 150 m-long beamline ID19. Micro-CT was successfully applied to characterise various scientific and industrial specimens. The main applications are originating from materials sciences, biomedical research and palaeontology. Due to the available high photon flux density, (specially in pink beam -polychromatic-mode, using either a single-harmonic undulator or filtered white beam), a strong demand is emerging employing this potential for time-resolved in situ experiments. Indirect detectors equipped with CMOS-based cameras have been successfully used for high speed imaging (one 3D image in 1s). Samples can be investigated in situ, employing different sample environments like tensile stress, compression, fatigue devices, low or high temperature, hygrometry control.

8:05 PM
X-ray Dark Field Microscopy: Henning Poulsen[1]; *Andrew King*[2]; Wolfgang Ludwig[2]; Anatoly Snigirev[2]; [1]Risoe DTU; [2]ESRF

We propose a new technique: x-ray dark field microscopy for mapping grains and their crystallographic properties in 3D and 4D. Conceptually similar to in-line dark field imaging in the TEM, the imaging principle involves the use of an objective - a so-called compound refractive x-ray lens. 3D information is obtained by means of tomographic reconstruction principles. In comparison to TEM much thicker specimens can be used comprising up to 50 grains across the specimen, Orientations and strain can be mapped in one (sub)grain at the time with a resolution of 0.001 deg and 10^-4 respectively. The spatial resolution is limited by the quality of the x-ray optics, which currently is of order 200 nm. We present a first demonstration experiment on Si and discuss the potential of the method in comparison to other 3D structural characterization tools such as 3DXRD, DAXM and serial sectioning.

8:25 PM Break

8:45 PM CANCELLED
Characterization of Orientation and Elastic Strain Gradients Inside Bulk Grains by Means of X-ray Diffraction Imaging Techniques: *Wolfgang Ludwig*[1]; Andrew King[2]; Peter Reischig[2]; Nicola Vigano[1]; Laura Nervo[2]; [1]Université de Lyon; [2]ESRF

Using a combination of X-ray diffraction contrast tomography, X-ray section and pinhole topography one can image weak orientation and elastic strain gradients inside individual bulk grains. The acquisition of diffraction images at close to 90 degree scattering angle offers enhanced resolution, both in real space and orientation space. This allows us to observe microstructural detail like slip bands and deformation twins, which are difficult to resolve in conventional forward scattering geometry. We will present first experimental results obtained from weakly deformed metallic samples made from Al and Mg alloys.

9:05 PM
Diffraction-Amalgamated Grain-Boundary Tracking (DAGT) Technique Applied to Al-3mass%Cu: *Darren LeClere*[1]; Takanobu Kamiko[1]; Masakazu Kobayashi[1]; Kentaro Uesugi[2]; Akihisa Takeuchi[2]; Yoshio Suzuki[2]; Hiroyuki Toda[1]; [1]Toyohashi University of Technology; [2]Japan Synchrotron Radiation Research Institute

By amalgamating X-Ray diffraction (XRD) microscopy with grain boundary tracking (GBT), a novel method which provides accurate analysis of individual grains during deformation has been created. Both, XRD and GBT are non-destructive techniques for in-situ characterizing of bulk materials, which allow for close to fracture analysis of metals. Employing near field XRD analysis, DAGT generates accurate information about individual grain orientations, whilst the GBT accesses submicron level analysis of grain morphologies in 3-dimensions. An X-ray pencil beam was employed for XRD analysis of an Al-3mass%Cu specimen, both before and after deformation. The morphology of each grain was determined by computer tomography (CT) imaging combined with liquid metal wetting; from which GBT provided an accurate description of the position and morphology of the grains. From this data, the algorithms developed for DAGT then identified which diffraction spots were related to which grain; consequently, providing a description of the misorientation between grains.

9:25 PM
X-ray Tomographic Microscopy at TOMCAT: Resolving the Dynamics of Materials: *Julie Fife*[1]; Rajmund Mokso[1]; Michel Rappaz[2]; Marco Stampanoni[3]; [1]Paul Scherrer Institut; [2]Ecole Polytechnique Fédérale de Lausanne; [3]Paul Scherrer Institut and ETH and University of Zurich

Non-destructive synchrotron X-ray tomographic microscopy is ideal for studying various materials systems in three and four dimensions, and the TOMCAT beamline of the Swiss Light Source is one of the premier beamlines in the world for such experiments. Spatial resolution ranges from 1-10µm with fields-of-view from 1-22mm and temporal resolution is as fast as 0.5s for full 3D data acquisition. Contrast varies from standard absorption, typically used in metal and composite systems, to propagation- and grating-based phase contrast, predominantly used for biological and other traditionally low-contrast materials. The efficient image-processing pipeline provides a full 3D reconstruction within seconds, making visualization close to real time. To exploit these state-of-the-art capabilities, dedicated systems have been developed to dynamically explore materials. This talk summarizes the capabilities at TOMCAT, specifically focusing on examples of elevated temperature processes, all observed in-situ, including solidifying and deforming metal ingots and mimicking volcanic processes in geomaterials.

9:45 PM
Measurement and Quantification of Grain Boundary Evolution in Three Dimensions during Grain Coarsening: *S. F. Li*[1]; B. W. Reed[1]; J. V. Bernier[1]; C. M. Hefferan[2]; J. Lind[2]; R. M. Suter[2]; M. Kumar[1]; [1]Lawrence Livermore National Lab; [2]Carnegie Mellon University

Microstructure measurements of polycrystalline samples have been traditionally limited to 2D surface techniques, which is unable to observe grain boundary motion within the bulk of a specimen. This is particularly problematic as grains often have complex, non-convex geometry and may intersect any given sample plane multiple times. This makes boundary motion estimates extremely difficult. To alleviate this problem, we have used the High Energy X-ray Diffraction Microscopy (HEDM), a non-destructive 3D orientation mapping technique to measure the microstructure of different anneal states of two copper specimens. From these volumetric orientation maps, grain boundaries, are extracted and tracked as the microstructure coarsens. A distribution of grain boundary motion as a function of boundary normal and misorientation is extracted, which allows us to examine the role of special boundaries during annealing. The effect of grain boundary topology is also quantified by comparing the motion of each of the samples.

Future Directions in 3D Materials Science

Thursday AM	Room: Exhibit Hall
July 12, 2012	Location: Seven Springs Mountain Resort

8:15 AM Invited
Exploiting Advances in Microscopy for Direct 3D Characterization of Materials: *Hamish Fraser*[1]; Daniel Huber[1]; John Sosa[1]; Brian Welk[1]; Robert Williams[1]; Peter Collins[2]; [1]The Ohio State University; [2]University of North Texas

An extremely important development has been the emphasis placed on Integrated Computational Materials Engineering (ICME) by the materials community. The development of accurate and precise computational approaches requires integration between characterization and modeling. This paper describes research aimed at developing accurate characterization methods, specifically direct 3D methods, which are applicable to a wide range of length scales, from atomic dimensions to the mesoscale. Several tools are required for this, including the RoboMetTM (optical scale), DualBeamTM FIB (SEM scale), STEM and EDS tomography (TEM scale), and the tomographical atom probe (atomic scale). Advances in each of these techniques will be described, and the accuracy of each technique will be assessed. This includes the performance of these techniques for the characterization of features, the scale of which corresponds to where these techniques overlap one another. This research has been supported in part by the US ONR.

8:45 AM Invited
The Five Parameter Grain Boundary Character Distribution of a TWIP Steel Determined from Three-dimensional Data Sets: Hossein Beladi[1]; *Gregory Rohrer*[2]; [1]Deakin University; [2]Carnegie Mellon University

Measuring, understanding, and controlling grain boundary anisotropy is critical to understanding and controlling microstructural evolution in polycrystalline materials. The grain boundary character distribution (GBCD) is defined as the relative areas of grain boundaries distinguished by lattice misorientation and grain boundary plane normal. Recently, the dual-beam focused ion beam (FIB) scanning electron microscope (SEM) has been used to automate the collection of serial sections of electron backscatter diffraction maps and the GBCD has been determined from these maps. In this talk, recent results from a TWIP steel will be compare to those of Ni. In general, we find that polycrystals with the same atomic structure have very similar GBCDs. The GBCDs also compare favorably to those of other fcc metals. Furthermore, the relative areas of different grain boundary types are inversely correlated to their energies.

9:15 AM Invited
A Workshop to Promote the Use of High-energy X-ray Diffraction Experiments and Detailed Computational Analyses for Understanding Multiscale Phenomena in Crystalline Materials: *Matthew Miller*[1]; Robert Suter[2]; Ulrich Lienert[3]; Armand Beaudoin[4]; [1]Cornell University; [2]Carnegie Mellon University; [3]Argonne National Laboratory; [4]University of Illinois at Urbana Champaign

High energy synchrotron x-ray diffraction methods have become important microstructural and micromechanical interrogation tools. The enormous potential for these probes lies in the ability to interface diffraction data with microstructure-based material models. This talk describes a workshop that was held in October, 2011 focusing on the interface between high energy x-ray methods and micromechanical modeling frameworks. Over thirty-five oral presentations were given by international experts who conduct synchrotron x-ray diffraction experiments, model material behaviors on multiple size scales or work in industry on relevant materials. The purpose of the workshop was to establish contacts and promote synergy between the various areas and to optimize the impact of the high value data by assuring that the most relevant and timely studies are performed and that these results can then serve as templates for experimental/theoretical collaborations in the future. A poster session for young researchers was also featured.

9:45 AM Break

10:00 AM Invited
Future Directions for 3D Imaging in the (S)TEM: *Paul Midgley*[1]; [1]University of Cambridge

In the past decade, electron tomography (ET) in the (S)TEM has moved from a niche technique to a standard materials science tool for 3D imaging and analysis at the nanoscale. In this presentation, I will review the current state-of-the-art focussing on recent developments including the application of ET to study nanoparticles with atomic resolution, the combination of 3D imaging and energy loss spectroscopy and the improved quantification of tomograms. Whilst improvements in hardware (e.g. aberration correctors) has aided development, some of the most significant progress recently has been in the implementation of novel reconstruction algorithms, incorporating a priori information to improve the fidelity of 3D reconstructions. This talk will highlight these and illustrate their benefits with reference to key materials problems. A look to the future will conclude the talk with suggestions (and challenges!) as to how ET may be used to explore new directions in 3D materials science.

10:30 AM Invited
3D Materials by Design: From Genome to Flight: *Greg Olson*[1]; [1]Northwestern University

Building on a system of fundamental databases now known as the Materials Genome, parametric materials design has integrated materials science, applied mechanics and quantum physics within a systems engineering framework to create a first generation of designer "cyberalloys" that have now entered commercial applications, and a new enterprise of commercial materials design services has steadily grown over the past decade. The success of computational materials design in the 1990s established a basis for the DARPA-AIM initiative of the 2000s which broadened computational materials engineering to address acceleration of the materials development and qualification cycle. A new level of science-based AIM modeling accuracy has now been achieved under the ONR/DARPA "D3D" Digital Structure consortium using a suite of advanced 3D tomographic characterization tools to calibrate and validate a set of high fidelity explicit 3D microstructural simulation tools spanning the hierarchy of microstructural scales, addressing strength, toughness and fatigue resistance.

11:00 AM Invited
The Critical Role of Digital 3D Structure in Advanced Materials Research and Development: *Julie Christodoulou*[1]; [1]Office of Naval Research

Descriptions of microstructure and understanding of mechanisms of microstructural evolution and response to external loads (thermal, mechanical, magnetic, et al.) has always been the center of materials science. As our characterization tools have enabled more precision, we have learned that descriptions of microstructure in 3D are often needed to describe realistic three-dimensional behavior. Work reported at this conference illustrates that acquiring 3D characterizations and understanding processing-structure-relationships in 3D are more challenging and data intensive efforts than our more conventional work. Compounding this, if we are to realize truly integrated approaches to materials research, development and implementation, these descriptions whether in 2 or 3D must be "digital", i.e. quantitative and precise. The implications of this observation on efforts to build digital products of materials research will be explored in the context of the Materials Genome Initiative and ICME.

11:30 AM Panel Discussion

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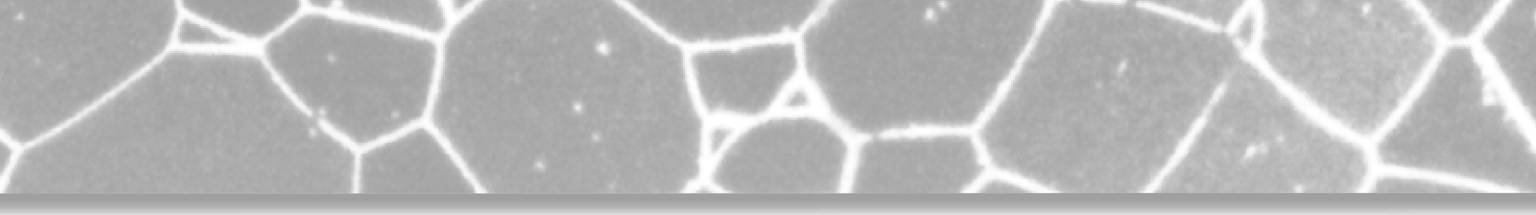

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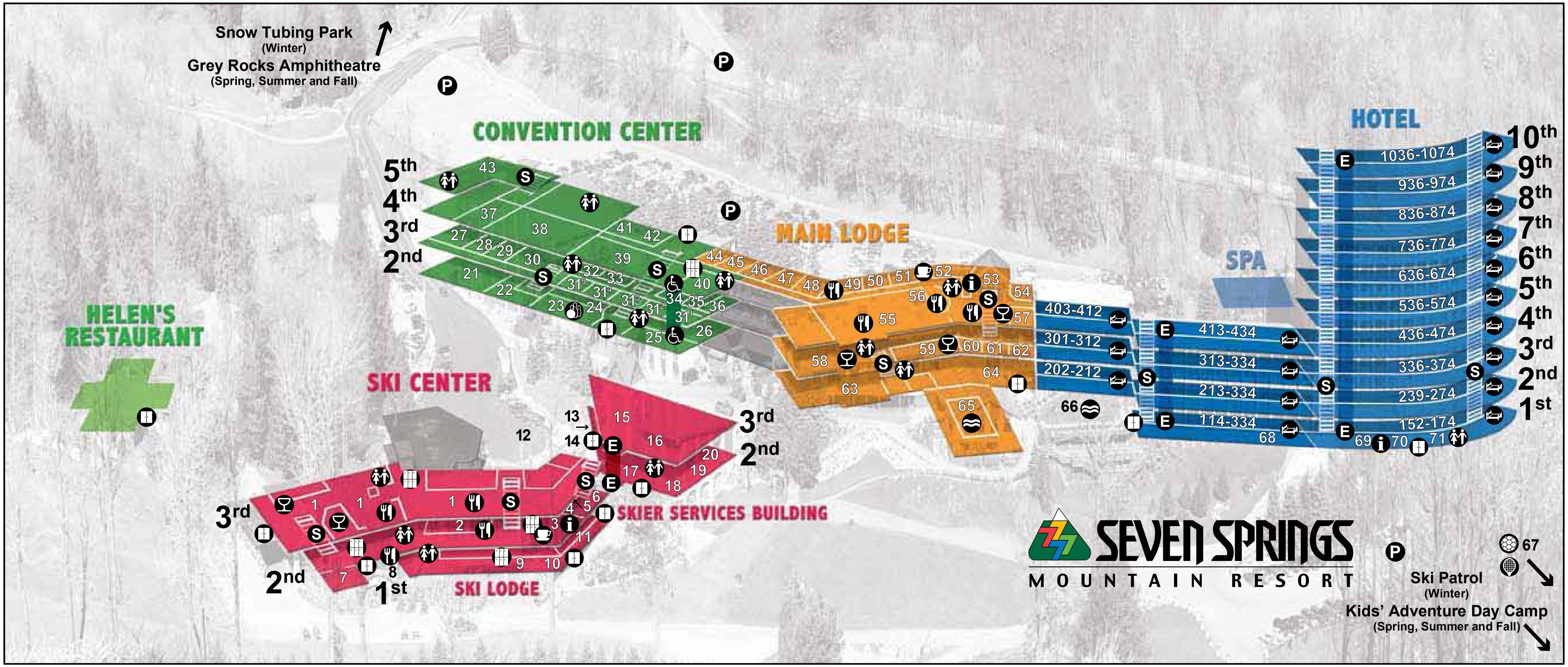

SKI CENTER

Ski Lodge
1. Foggy Goggle
2. Snowbase Café
3. Mountain Perk
4. Mountain Memories Photography
5. Snow Base Shoppe
6. Maple Room
7. Ski Check
8. Emo's Pit
9. Coin Lockers
10. Junior Snowsports School
11. Rental Shop

Skier Services Building
12. Shuttle Pick-up for Parking Lot
13. Season Pass and Group Ticket Office
14. Ski/Board Ticket Office
15. Timberstone Room (Spring and Summer)
16. Willi's Ski Shop (Fall and Winter)
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CONVENTION CENTER
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22. Exercise Room
23. Bowling Center
24. Cub Trap Game Room
25. Fox Den
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27. Dogwood Forum
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56. Dragonfly Café
57. Bavarian Lounge
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60. Resort Realty
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63. Miniature Golf
64. Bear Trap Game Room
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67. Tennis and Volleyball Courts

HOTEL
68. Ski Trips Office
69. Hotel Service
70. Shoppe at the Springs
71. Hotel Registration

Entrance · Restrooms · Stairs · Elevators · Handicap Elevator · Room · Service/Information · Mountain Perk · Restaurant · Bar · Pool · Tennis Courts · Bowling · Volleyball · Lockers · Parking

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