The 4th International Congress on

3DMS

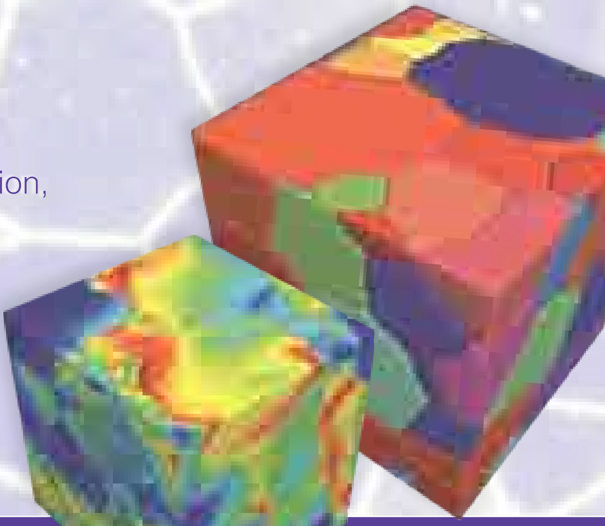
3D Materials Science 2018

June 10–13, 2018
Kulturværftet (Culture Yard) Conference Center
Helsingør (Elsinore), Denmark

FINAL PROGRAM

Sponsored by:

TMS and the TMS Advanced Characterization, Testing & Simulation Committee



www.tms.org/3DMS2018

SCHEDULE OF EVENTS

Please note that all times are in Central European Summer Time (CEST) +0200 UTC.

Sunday, June 10	Time	Location
Registration	5:00 p.m. to 7:30 p.m.	Outside Salon, Beach Hotel Marienlyst
Welcome Reception	6:30 p.m. to 7:30 p.m.	Salon, Beach Hotel Marienlyst

Monday, June 11	Time	Location
Registration	7:00 a.m. to 6:00 p.m.	Arcade, Prismen
Keynote	8:00 a.m. to 9:00 a.m.	Store Scene
Technical Sessions	9:00 a.m. to 10:00 a.m.	(See technical program)
Break	10:00 a.m. to 10:30 a.m.	Arcade, Prismen
Poster & Exhibit Set-Up	10:00 a.m. to 10:30 a.m.	Store Scene
Technical Sessions	10:30 a.m. to 12:10 p.m.	(See technical program)
Lunch	12:10 p.m. to 1:30 p.m.	On your own
Technical Sessions	1:30 p.m. to 3:20 p.m.	(See technical program)
Break; Exhibit Viewing	3:20 p.m. to 3:50 p.m.	Store Scene
Technical Sessions	3:50 p.m. to 6:20 p.m.	(See technical program)
Poster Reception & Exhibit Viewing	6:30 p.m. to 7:30 p.m.	Store Scene

Tuesday, June 12	Time	Location
Registration	7:30 a.m. to 6:00 p.m.	Arcade, Prismen
Keynote	8:00 a.m. to 9:00 a.m.	Store Scene
Technical Sessions	9:00 a.m. to 10:00 a.m.	(See technical program)
Break; Exhibit Viewing	10:00 a.m. to 10:30 a.m.	Store Scene
Technical Sessions	10:30 a.m. to 12:10 p.m.	(See technical program)
Lunch	12:10 p.m. to 1:30 p.m.	On your own
Technical Sessions	1:30 p.m. to 3:20 p.m.	(See technical program)
Break; Exhibit Viewing	3:20 p.m. to 3:50 p.m.	Store Scene
Technical Sessions	3:50 p.m. to 6:20 p.m.	(See technical program)
Dinner Event	6:30 p.m. to 8:30 p.m.	Kadetten at Kronborg

Wednesday, June 13	Time	Location
Registration	7:30 a.m. to 4:20 p.m.	Arcade, Prismen
Technical Sessions	8:00 a.m. to 9:50 a.m.	(See technical program)
Break; Exhibit Viewing	9:50 a.m. to 10:20 a.m.	Store Scene
Technical Sessions	10:20 a.m. to 12:10 p.m.	(See technical program)
Lunch	12:10 p.m. to 1:30 p.m.	On your own
Poster & Exhibit Tear-Down	12:10 p.m. to 1:30 p.m.	Store Scene
Technical Sessions	1:30 p.m. to 3:20 p.m.	(See technical program)
Break	3:00 p.m. to 3:20 p.m.	Store Scene
Closing Keynote	3:20 p.m. to 4:20 p.m.	Store Scene

Thursday, June 14	Time	Location
Max IV Laboratory Tour	11:00 a.m. to 6:00 p.m.	Off-Site

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WELCOME TO

The 4th International Congress on 3DMS

3D Materials Science 2018

On behalf of The Minerals, Metals & Materials Society (TMS), we are pleased to welcome you to the fourth iteration of the International Congress on 3D Materials Science (3DMS 2018). This multi-disciplinary meeting distills the most current knowledge regarding 3D materials science into one conference, enabling you to fast-forward your materials research impact. We hope you will take every opportunity during this week to immerse yourself in this unique, highly focused technical meeting where you have the chance to learn from and network with other 3D materials science experts. The 3DMS 2018 technical program will include plenary and invited lectures as well as oral and poster presentations including a wide range of topic areas, covering the most critical and rapidly growing areas of 3D materials science.

We look forward to an exciting congress and thank you for your participation in 3DMS 2018!

Warmest regards from the organizing committee:

ORGANIZING COMMITTEE

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Technical University of Denmark (DTU), Denmark

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Please note that all times are in Central European Summer Time (CEST) +0200 UTC.

REGISTRATION

Your registration badge ensures admission to each of these events:

- Technical and poster sessions
- Sunday welcome reception
- Monday poster reception
- Tuesday dinner event*
- Refreshment breaks during session intermissions

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

REGISTRATION HOURS

On Sunday, June 10, the registration desk will be located outside the Salon at the Beach Hotel Marienlyst at the following times:

Sunday	**5:00 p.m. to 7:30 p.m.**

From Monday, June 11, through Wednesday, June 13, the registration desk will be located in Arcade, Prismen, at the Kulturværftet (Culture Yard) Conference Center at the following times:

Monday	**7:00 a.m. to 6:00 p.m.**
Tuesday	**7:30 a.m. to 6:00 p.m.**
Wednesday	**7:30 a.m. to 4:20 p.m.**

TECHNICAL SESSIONS

All oral presentations will be held in the Store Scene and Lille Scene at the Kulturværftet (Culture Yard) Conference Center. All poster presentation will be held in the Store Scene. See the Technical Program section on pages 11–43 for room locations.

INTERNET ACCESS

Complimentary internet access is available for attendees in some public areas of the hotel and in all hotel guest rooms. Complimentary internet access is also available at the Kulturværftet (Culture Yard) Conference Center. The username is KV-publikum and no password is required.

EXHIBITION HOURS

The exhibition will be located in Store Scene at the Kulturværftet (Culture Yard) Conference Center.

Monday	**3:20 p.m. to 3:50 p.m. and 6:30 p.m. to 7:30 p.m.**
Tuesday	**10:00 a.m. to 10:30 a.m. and 3:20 p.m. to 3:50 p.m.**
Wednesday	**9:50 a.m. to 10:20 a.m.**

WELCOME RECEPTION

The Welcome Reception will be held on Sunday, June 10, from 6:30 p.m. to 7:30 p.m. in the Salon at the Beach Hotel Marienlyst.

POSTER RECEPTION

A networking reception for poster and exhibit viewing is planned for Monday, June 11, from 6:30 p.m. to 7:30 p.m. in the Store Scene at the Kulturværftet (Culture Yard) Conference Center. Don't miss this great networking opportunity!

CONGRESS DINNER

The 3DMS 2018 dinner event will be held on Tuesday, June 12, from 6:30 p.m. to 8:30 p.m. Please note that while one ticket for the congress dinner is included, registration was required for this event through the congress registration form. Onsite ticket sales are based on availability. Check with TMS staff at the registration desk for more information.

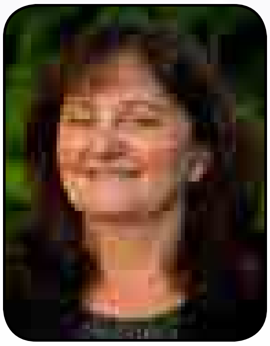
ABOUT THE VENUE

KULTURVÆRFTET (CULTURE YARD) CONFERENCE CENTER

The Kulturværftet (Culture Yard) Conference Center, the congress program location, is a multi-cultural house situated in Helsingør (Elsinore)—a historic town at the top of North Zealand overlooking the strait between Denmark and Sweden. Built into the town's old shipyard, the Culture Yard gives you every opportunity to explore the vibrant culture of Elsinore. For more information, visit https://kuto.dk.

BEACH HOTEL MARIENLYST

The Beach Hotel Marienlyst, the congress hotel and Sunday reception and registration location, is a 4-star seaside hotel complete with a spa, casino, and wellness area. It offers its own dining options and is also situated near central Elsinore, where you can find an assortment of other shopping and dining options. Also within walking distance are wooded trails, a small boat marina, and the historic Kronborg Castle, the setting for Shakespeare's *Hamlet*. For more information, visit www.marienlyst.dk/en.home/.



Tresa M. Pollock, University of California, Santa Barbara
Presentation Title: "Challenges in Acquisition of Statistically Significant Multimodal 3D Data for Property Prediction"
About the Speaker: Tresa M. Pollock is the Alcoa Professor of Materials at the University of California, Santa Barbara. She graduated with a B.S. from Purdue University in 1984, and a Ph.D. from Massachusetts Institute of Technology in 1989. Pollock was employed at General Electric Aircraft Engines from 1989 to 1991, where she conducted research and development on high temperature alloys for aircraft turbine engines. She was a professor in the Department of Materials Science and Engineering at Carnegie Mellon University from 1991 to 1999 and the University of Michigan from 2000 to 2010. Her current research focuses on processing and properties of structural materials and coatings and on the use of ultrafast lasers for microfabrication, tomography and materials diagnostics. Pollock was elected to the U.S. National Academy of Engineering in 2005, is a Fellow of TMS and ASM International, serves as principal of the Metallurgical and Materials Transactions family of journals, and was the 2005 TMS President.

Henry Proudhon, Mines Paristech, Centre des Matériaux
Presentation Title: "Polycrystalline Materials in 4 Dimensions"
About the Speaker: Henry Proudhon graduated in 2001 from École Centrale de Lyon in France in mechanical engineering. He received his Ph. D. in material science in 2005 from INSA Lyon working on investigating fatigue cracking mechanisms with synchrotron x-ray tomography. He then went to the University of British Columbia to work with Warren Poole on ultrafine-grained materials and the Bauschinger effect. In 2007, he joined CNRS, the French national research institute for science, at Centre des Matériaux MINES ParisTech to carry out his research on three dimensional study of deformation and fracture in polycrystalline materials: from synchrotron x-ray investigations to computational mechanics. In 2015 he defended his habilitation thesis and also was associated to the DiffAbs beamline at the SOLEIL synchrotron near Paris. Last year he was a visiting researcher at the University of California, Santa Barbara in Tresa Pollock's research group, to work on Ni-based superalloys and TiAl alloys. Back in Europe, he continues to work to improve structural materials with partners like Safran, Dassault Aviation or Arkema. He has coauthored more than 50 publications in international peer reviewed journal and received several award such as the FEMS/TMS Young Leaders International Scholar award in 2016.

Stéphane Roux, National Center for Scientific Research
Presentation Title: "Imaging Mechanical Models"
About the Speaker: Stéphane Roux graduated from École Polytechnique in 1983 and the École Nationale des Ponts et Chaussées (ENPC) in 1985. He received his Ph.D. in mechanical engineering from the ENPC in 1990. As a CNRS research professor, he was successively at École Supérieure de Physique et Chimie Industrielles de la Ville de Paris (ESPCI), at the joint CNRS/Saint-Gobain Research Laboratory, and currently, he is at the Laboratory of Mechanics and Technology at École Normale Supérieure de Paris-Saclay. Roux holds seven patents, and is the author of more than 350 publications. In 2006, he received the Silver Medal in Information and Engineering Sciences from the CNRS. His current research activities are in theory at the service of experimental mechanics—the development of image-based measurements in solid mechanics, aimed to deliver quantitative evaluation of mechanical properties with the least uncertainties.

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

PLATINUM SPONSOR

ZEISS Microscopy is the world's only one-stop manufacturer of light, electron, X-ray, and ion microscope systems and offers solutions for correlative microscopy. The portfolio compromises products and services for the life sciences and materials research as well as for industry, education and clinical practice. The business group is headquartered in Jena. Additional production and development sites are located in Oberkochen, Göttingen, and Munich, as well as in Cambridge in the UK, and in Peabody, MA, and Pleasanton, CA, in the USA. The business group is allocated to the Research & Quality Technology segment. Around 6,300 employees work for the segment, generating revenue totaling €1.5 billion in fiscal year 2016/17.

SILVER SPONSOR

Xnovotech Technology ApS specializes in the development of innovative 3D X-ray imaging solutions for engineers and scientists with emphasis on 3D crystallographic imaging tools for applications within engineering, materials sciences and geosciences. The 3D crystallographic imaging solution GrainMapper3D™, available as part of the LabDCT™ module on the ZEISS Xradia 520 Versa X-ray Microscope, enables non-destructive studies of microstructural evolution in the home lab. With full access to 3D grain morphology and crystallographic orientations, GrainMapper3D opens unique possibilities for the study of damage, deformation and growth mechanisms related to 3D materials science.

BRONZE SPONSORS

Bruker microCT develops and produces a wide range of high-end nano- and micro-tomography instruments for material research, life science and in-vivo preclinical studies. Building on more than thirty-five years' experience, Bruker microCT made the first commercial desktop microCT scanner in 1996. Today our SkyScan scanners reach a spatial resolution in the sub-micron range. Bruker microCT is part of the Bruker Corporation, a global market and technology leader in materials research, life science and quality control instrumentation. Our goal is enabling scientists to make breakthrough discoveries and develop new applications that improve the quality of human life. Today, worldwide more than 6,000 employees are working on this permanent challenge at over 90 locations on all continents.

Volume Graphics develops leading software for the analysis and visualization of industrial computed tomography (CT) data. Software like the extendable high-end solution VGSTUDIO MAX help companies find out as much about their products as possible—and non-destructively at that. In 2016, for example, more than 70% of the "Fortune Global 500" companies worldwide in the automotive and electronics industries were using Volume Graphics solutions for quality control, metrology, damage analysis, and product development. Industrial CT provides the basis for this, as CT scans reveal every aspect of a component. Volume Graphics was founded in 1997 in Heidelberg, Germany, where our headquarters still are today. Subsidiaries are located in the USA, Japan, China, and Singapore.

Bronze and Tabletop Sponsors Continued on Next Page

XRE is a new alternative for 3D X-ray imaging - Dynamic solutions for your lab. Founded as a spinoff from Ghent University in Belgium, XRE develops leading-edge 3D X-ray micro-computed tomography (micro-CT) systems designed to meet specific application demands, combined with a suite of software solutions that facilitate 3D image acquisition, reconstruction, visualization, quantification and collaboration. XRE's micro-CT products, UniTOM, CoreTOM and DynaTOM, exhibit leadership in dynamic micro-CT imaging in the laboratory, enabling the study of materials evolution under various sample environments (in situ). Such non-destructive imaging technologies have proven essential for research markets including materials research, geosciences, industrial parts, life sciences and others. In March 2018, XRE proudly became part of TESCAN, a leading global supplier of microscopy systems, via acquisition. This will accelerate XRE's ability to serve a growing international micro-CT community.

TABLETOP SPONSOR

Math2Market GmbH from Kaiserslautern was spun off six years ago from the Fraunhofer Institute for Industrial Mathematics (ITWM) in Kaiserslautern. The founders of the company are also the developers of the scientific software GeoDict - The Digital Material Laboratory, developed and distributed by Math2Market GmbH and already bearing this name since 2001. Our company, with its innovative ideas and close cooperation with its customers, has managed to continuously improve the software and increase the number of employees to around 40. Through our dedicated, competent employees and distributors in America and Asia, we offer our more than 150 customers worldwide personal contacts. They are happy to advise and support you in your research and development questions.

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

REFUNDS
The deadline for all refunds was May 8, 2018. No refunds will be issued at the congress. Fees and tickets are nonrefundable.

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

ATTENDEES WITH DISABILITIES

TMS is headquartered in the United States of America and complies with the Americans with Disabilities Act (ADA) for all events. The ADA prohibits discrimination against, and promotes public accessibility for, those with disabilities. We ask those requiring specific equipment or services to contact TMS Meeting Services at mtgserv@tms.org in advance.

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

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

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

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

PHOTOGRAPHY AND RECORDING

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

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

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

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

EMERGENCY PROCEDURES

The chances of an emergency situation occurring at 3DMS 2018 are quite small. However, being prepared to react effectively in case of an incident is the most critical step in ensuring the health and safety of yourself and those around you. Please take a few moments to review the maps of the Beach Hotel Marienlyst and the Kulturværftet (Culture Yard) Conference Center printed in this program (on page 51). When you enter each building, familiarize yourself with the exits and the stairs leading to those exits. When you arrive at your session or event location, look for the emergency exits that are in closest proximity to you.

In case of a fire at the Kulturværftet (Culture Yard) Conference Center, all attendees will be advised in Danish and English to leave the building through the nearest fire exit. The staff at the Culture Yard is trained to get their guests out of the building, and there is a fully automatic fire warning system.

In case of an emergency, contact one of the Culture Yard staff members who will contact the appropriate authority. The emergency number in Denmark is 1–1–2 (corresponding to 9–1–1 in the United States).

STAYING FOR THE TOUR?

Please note that all times are in Central European Summer Time (CEST) +0200 UTC.

If you registered for the **Max IV Laboratory Tour**, please note the following important information:

When: Thursday, June 14, 2018
Where: Lund, Sweden
Departure Time: Depart from Beach Hotel Marienlyst at 11:00 a.m.
Return Time: Arrive at Beach Hotel Marienlyst at 6:00 p.m.

Registration includes transportation to and from Beach Hotel Marienlyst and a tour of the Max IV facility. For more information on the Max IV Laboratory, visit the Lab Tour page at www.tms.org/3DMS2018.

Please note that the deadline to register was May 28, 2018. Tickets for this event can no longer be purchased.

MAX IV

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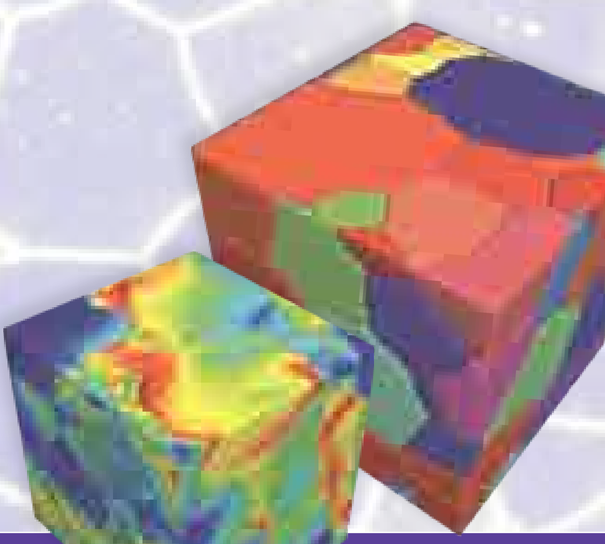
TECHNICAL PROGRAM

www.tms.org/3DMS2018



Monday Plenary

Monday AM
June 11, 2018

Room: Store Scene
Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

8:00 AM Plenary

Imaging Mechanical Models: *Stéphane Roux*[1]; [1]ENS Paris-Saclay/CRNS/University Paris-Saclay

Digital Volume Correlation (DVC) consists in a non-rigid registration of 3D images of materials. When successive images of a specimen under load are processed, space-time displacement can be measured, and from them mechanical properties can be inferred through mechanical identification. Tomographic image reconstruction, DVC and identification are three inverse problems that share a number of similarities. Moreover they can be combined by pairs and even into a single procedure with radiographs as input and mechanical properties as output. The fusion of these operations results in a net gain in fidelity and efficiency, allowing kinematic or mechanical models to be used as regularizations to help solving the inverse problem. Additionally, it also opens the door to model reduction techniques to further optimize the entire process. This "grand unification" will be illustrated through different examples showing that a mechanical test classically performed in one week, can be completed in a few minutes with a similar quality.

8:45 AM Question and Answer Period

9:00 AM Break

New Experimental and Analysis Methods I

Monday AM
June 11, 2018

Room: Lille Scene
Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

9:10 AM Invited

Advances in Neutron Imaging for Bulk Microstructure Investigations and Future Capabilities at the European Spallation Source: *Robin Woracek*[1]; Nikolay Kardjilov[2]; Andre Hilger[2]; Markus Strobl[3]; Anton Tremsin[4]; [1]European Spallation Source; [2]Helmholtz Zentrum Berlin; [3]Paul Scherrer Institut; [4]University of California at Berkeley

The European Spallation Source in Lund, Sweden, will be the most powerful neutron source for materials research. Among the first eight instruments that start user operation in 2023 are the imaging beamline ODIN and the engineering diffractometer BEER. In order to unlock the tremendous potential from this long pulse neutron source for 3D material characterization, novel methods are under constant development. This presentation will outline the current and future possibilities of neutron imaging for engineering materials research at existing spallation and reactor sources. Recent scientific and methodological highlights obtained by the authors will be shown, including 3D phase mapping in rectangular TRIP steel under torsional deformation and visualization of hydrogen embrittlement and blistering in iron samples.

9:40 AM

3D Microstructural Mapping Using Neutron Time-of-flight Transmission Imaging: *Joe Kelleher*[1]; [1]Engin-X, ISIS, STFC

Electron, X-ray and neutron diffraction are widely recognised as complementary techniques, each best suited to a different range of length scales and sample materials. Of these, EBSD is now routinely used to map crystal orientations on a 2D surface and X-ray DCT can reconstruct microstructures in samples with sub-millimetre dimensions, but so far the potential of neutrons to map larger volumes remains relatively unexplored. A particular strength of neutron-based crystal orientation determination is the ability to use time-of-flight transmission spectra to obtain orientation for a crystallite from a small number of projections, which can also reduce the need to match up the grains visible in the transmitted data to diffraction spots outside the transmitted beam. Accordingly, we present a method for 3D microstructural mapping in a coarse-grained nickel superalloy that demonstrates the advantages of neutron based approach for this type of problem.

10:00 AM Break

10:30 AM

Three Dimensional Polarimetric Neutron Tomography of Magnetic Fields: *Morten Sales*[1]; Markus Strobl[2]; Takenao Shinohara[3]; Anton Tremsin[4]; Anders Dahl[5]; Søren Schmidt[1]; [1]Department of Physics, Technical University of Denmark; [2]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute; [3]J-PARC Center, Japan Atomic Energy Agency; [4]Space Sciences Laboratory, University of California at Berkeley; [5]Department of Applied Mathematics and Computer Science, Technical University of Denmark

We present our successful demonstration of Time-of-Flight Three Dimensional Polarimetric Neutron Tomography (ToF 3DPNT) for the non-destructive measurement and reconstruction of three dimensional magnetic field strengths and directions, a technique capable of extracting hitherto unmeasurable properties from bulk samples. Using a state-of-the-art polarimetric set-up for ToF neutron instrumentation at the J-PARC RADEN beamline, Japan, in combination with a newly developed reconstruction algorithm, we have measured and reconstructed the magnetic field generated by a current carrying solenoid.Furthermore, we present the current status of reconstruction techniques applicable to stronger magnetic fields such as those in a crystal with multiple magnetic domains. Such techniques utilise the ToF information in combination with a forward model to get around the issue of phase wrapping, where neutron precess by more than 180°.

10:50 AM

Fast In Situ Nanotomography at ESRF: *Julie Villanova*[1]; Richi Kumar[1]; Rémi Daudin[2]; Pierre Lhuissier[2]; David Jauffres[2]; Christophe L. Martin[2]; Rémi Tucoulou[1]; Luc Salvo[2]; [1]ESRF - The European Synchrotron; [2]SIMAP Univ. Grenoble Alpes-CNRS

In the framework of the European Synchrotron Radiation Facility (ESRF) upgrade program, the new nano-analysis beamline ID16B has been recently built to accommodate several micro-analytical techniques (XRF, XANES, XRD) combined with magnified tomography. The beamline configuration offers an improved lateral resolution (50 nm) and a larger flexibility capable of in-situ experiments. In this work, we present the development of a fast in situ nanoimaging set-up[1] that allows high temperature experiments to be performed with an unprecedented combination of nanometer pixel size (<100nm) and fast acquisition (<10s). Several on-going material investigations: ceramics sintering and light alloys high temperature mechanical deformation will illustrate the capabilities of the technique. We will discuss the actual challenges and limitations of this breakthrough in materials science in situ characterization as well as future possibilities offered by the EBS upgrade program at the ESRF.[1] J. Villanova et al., Materials Today 20 (2017), 354-359.

11:10 AM

Lensless Imaging with a Lens: *Anders Pedersen*[1]; Virginie Chamard[2]; Carsten Detlefs[3]; Henning Poulsen[1]; [1]Technical University of Denmark; [2]Institut Fresnel; [3]ESRF

Non-destructive characterization in 3D of polycrystals on all length scales is one of the grand challenges of materials science. X-rays have favorable properties, such as being able to penetrate bulk samples of relevant materials. We have earlier introduced 3DXRD/DCT and dark field microscopy that produces detailed maps of grains and domains with a resolution of 2 µm and 100 nm, respectively. Here we demonstrate a new technique capable of imaging small regions inside mm-sized bulk samples with a spatial resolution of 20 nm. To allow this we utilize coherent X-ray diffraction in combination with an objective lens. We present simulated data that shows better resolution than a standard imaging setup and is more resilient against lens manufacturing errors. We will introduce the method, show preliminary experimental results, and discuss its applications in materials science.

11:30 AM
In Situ High-temperature X-ray Microtomography at the Elettra Synchrotron Facility Using a Newly Designed Induction Furnace: *Marko Kudrna Prasek*[1]; Mattia Pistone[2]; Don Baker[1]; Nicola Sodini[3]; Nicoletta Marinoni[4]; Gabriele Lanzafame[3]; Lucia Mancini[3]; [1]McGill University; [2]University of Lausanne (UNIL); [3]Sincrotrone Trieste S.C.p.A.; [4]Università degli Studi di Milano

An induction furnace was designed for in situX-ray microtomography (mCT) at the SYRMEP beamline of Sincrotrone Elettra, with special attention placed on flexibility, precise temperature control and the ability to operate for long durations, -all crucial for many materials science and geoscience applications. We present several applications of this furnace: 1) Platinum (Pt) nugget growth was studied at high-temperature due to the importance of Pt ore deposits in rocks and Pt nuggets in glass synthesis; 2) Plagioclase nucleation and growth was investigated at high temperature due to the presence of plagioclase in many rock-types; And, 3) clays were studied during firing to track their reactions during the high temperature treatment used to produce ceramics. In situ high-resolution synchrotron X-ray mCT studies with this type of furnace combined with the potential of phase-contrast imaging are a newly available and highly promising tool to study high-temperature processes in materials directly in 3D.

11:50 AM
Mapping Grain Morphology and Orientation by Laboratory Diffraction Contrast Tomography: Nicolas Gueninchault[1]; Florian Bachmann[1]; Hrishikesh Bale[2]; Kenneth Nielsen[1]; Jun Sun[1]; Christian Holzner[1]; Leah Lavery[2]; *Erik Lauridsen*[1]; [1]Xnovo Technology ApS; [2]Carl Zeiss X-ray Microscopy Inc

Recent developments of the Laboratory Diffraction Contrast Tomography (LabDCT) technique have extended its capabilities to include full reconstruction of the 3D grain structure, including both grain morphology and crystallographic orientation. LabDCT makes use of high-resolution diffraction images acquired on a ZEISS Xradia 520 Versa X-ray microscope. The diffraction signals are based on polychromatic X-rays and acquired in a special Laue-focusing geometry that helps increase the signal-to-noise ratio. The 3D crystallographic imaging capabilities of LabDCT complements the structural data obtained by traditional absorption-based tomography and together they provide unprecedented insight into materials structure. We will present a selection of LabDCT results with particularly emphasis on its non-destructive operation. We will discuss boundary conditions of the current implementation, compare with conventional synchrotron approaches, point to the future of the technique and discuss ways in which this can be correlatively coupled to related techniques for better understanding of materials structure evolution in 3D.

Phase Transformations, Particle Coarsening, Grain Growth, and Recrystallization I

Monday AM
June 11, 2018

Room: Store Scene
Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

9:10 AM Invited
Application of Characterization, Modelling, and Analytics towards Understanding Process-structure Linkages in Metallic 3D Printing: *Michael Groeber*[1]; [1]Air Force Research Laboratory

We will present methods for combining process monitoring, thermal modeling and microstructure characterization together to draw process-to-structure relationships in metal additive manufacturing. The talk discusses heterogeneities in the local processing conditions within additively manufactured components and how they affect the resulting material structure. Methods for registering and fusing disparate data sources are presented and some effort is made to discuss the utility of different data sources for specific microstructural features of interest. The talk will highlight the need for improved understanding of metallic additive manufacturing processes and show that combining experimental data with modelling and advanced data processing and analytics methods will accelerate that understanding.

9:40 AM
Dark Field X-ray Microscopy Study of Heat Treatment of Fe-Si and Fe-Si-Sn Alloys: *Can Yildirim*[1]; Nikolas Mavrikakis[2]; Melanie Gauvin[3]; Phil Cook[1]; Mustafacan Kutsal[1]; Ashley Bucsek[4]; Henning Poulsen[5]; Wahib Saikaly[3]; Roger Hubert[3]; Carsten Detlefs[1]; [1]European Synchrotron Radiation Facility; [2]Aix-Marseille University, Institut Matériaux Microélectronique Nanosciences de Provence-IM2NP; [3]Onderzoeks Centrum voor de Aanwending van Staal; [4]Colorado School of Mines; [5]Technical University of Denmark

Properties of engineering materials can be improved by controlling various microstructural developments in heat treatment processes. Here, we study the effect of Sn in recovery and recrystallization of cold rolled Fe-3%Si binary and Fe-3%Si-0.1%Sn ternary alloys by means of 3D X-ray diffraction (3DXRD) and dark field X-ray microscopy (DFXM). DFXM is a non-destructive technique that allows 3D mapping of orientation and lattice strain with 100 nm spatial and 0.001° angular resolution within individual grains embedded in bulk samples. We investigate grains with the <111> direction parallel to the normal direction of cold rolling. Surprisingly, the recrystallized grains in both binary and ternary alloys show internal low angle boundary networks. We discuss the role of Sn during recovery and how it affects the subsequent recrystallization process. Our results also show that deformed grains feature sub-micron size deformation bands both in as-cold rolled and recovered states.

10:00 AM Break

10:30 AM
Understanding the Relationship Between Microstructure Evolution and Macroscopic Behavior in NiTi Martensite Reorientation: *Ashley Bucsek*[1]; Darren Pagan[2]; Darren Dale[2]; J.-Y. Peter Ko[2]; Aaron Stebner[1]; [1]Colorado School of Mines; [2]Cornell High Energy Synchrotron Source

Together with phase transformation, the diffusionless rearrangement of crystallographic twins enables the functional behaviors of the vast majority of ferroic and multiferroic materials. As a result, understanding twin mobility is critical to the success of a wide variety of society-improving technologies driven by ferroic and multiferroic materials. In the case of ferroelastic alloys, or shape memory alloys (SMAs), the mobile twins exist in the martensite phase and is thus referred to as martensite reorientation. As a study into twin reorientation, we performed stress-induced reorientation experiments on martensitic NiTi SMAs using near-field and far-field 3D X-ray diffraction (3DXRD) and digital image correlation (DIC). The results reveal the microstructure evolution behind two types of macroscopic localized deformation bands. These bands proceed through the sample in sequence, exist on a specific crystallographic plane, and both result in and are assisted by the elastic misorientation of the lattice.

10:50 AM

Understanding Grain Growth in 3D: Microstructural Evolution of Nickel during Multiple Annealing Stages Using Three-dimensional X-ray Microscopy: *Aditi Bhattacharya*[1]; C.M. Hefferan[2]; S-F. Li[3]; J. Lind[4]; Y-F. Shen[1]; R.M. Suter[1]; G.S. Rohrer[1]; [1]Carnegie Mellon University; [2]R. J. Lee Group; [3]Ditto Inc.; [4]Lawence Livermore National Laboratory

Near-field High Energy X-ray Diffraction Microscopy(nf-HEDM), a non-destructive, synchrotron based 3D characterization technique was used to track the microstructural evolution of high purity polycrystalline Nickel annealed at 800°C and measurements were taken at five different times separated by 30 minute intervals. The temporal changes in crystallographic orientation, grain size and misorientation in the microstructure were measured over the different anneal states. Our algorithm tracks each grain during annealing and matches them based on orientation and spatial location, thereby allowing detailed analysis of the grain boundary (GB) character distribution, the relative GB energies, and the GB curvature distribution at each step during the interrupted thermal annealing. Our results have been compared with established theories of grain growth and we discuss the topological nature of grain boundary network like the Aboav-Weaire law, but in 3D. The present work attempts to demonstrate a correspondence between a grain's growth trajectory and its neighborhood.

11:10 AM

Nanoscale 4D Microstructural Evolution of Precipitates in Aluminum Alloys using Transmission X-ray Microscopy (TXM): C. Shashank Kaira[1]; Tyler Stannard[1]; Vincent De Andrade[2]; Francesco De Carlo[2]; *Nikhilesh Chawla*[1]; [1]Arizona State University; [2]Advanced Photon Source

The complex distribution of different precipitate morphology can play a significant role in controlling the mechanical response of precipitation-strengthened alloys. It is well known that conventional characterization techniques like transmission electron microscopy and atom probe tomography have significant shortcomings in terms of their destructive nature and inability to sample a statistically relevant region. In this study, 3D X-ray nanotomography using Transmission X-ray Microscopy (TXM) has been employed to quantify, in detail, the evolution of the microstructure in an Al-3.5Cu alloy. Owing to its high spatial resolution, non-destructive nature and quick acquisition time, high temperature in situ studies were conducted to better understand the aging phenomena and the transformation reactions involved, in 3D. This technique was coupled with techniques like EBSD and micropillar compression, that allowed us to establish accurate structure-property relationships to better predict the alloy's deformation behavior.

11:30 AM

Parameter Estimation for Multi-phase-field Simulation Using Ensemble Kalman Filter: *Akinori Yamanaka*[1]; Yuri Maeda[1]; Kengo Sasaki[1]; [1]Tokyo University of Agriculture and Technology

In order to simulate the microstructure evolutions quantitatively using the multi-phase-field (MPF) model, we need to identify material parameters used in the MPF simulations from experimental data. Recently, direct observation of microstructure evolution processes has been possible using new experimental techniques like X-ray tomography. If the material parameters used for the MPF simulations can be estimated from the data obtained by such experimental techniques, the accuracy of the MPF simulations will be significantly improved. In this study, we propose a data assimilation (DA) methodology for estimating material parameters used for the 3D MPF simulation using the ensemble Kalman Filter (EnKF). The EnKF-based DA methodology is applied to estimate the anisotropic grain boundary mobility used in the 3D MPF simulation of polycrystalline grain growth. In this presentation, we show that our DA methodology can estimate the cusp of grain boundary mobility from a time-evolving 3D polycrystalline grain distribution.

11:50 AM

The Dynamics of Complex Two-phase Mixtures During Coarsening: From Dendritic to Bicontinuous Mixtures: Yue Sun[1]; William Andrews[2]; Katsuyo Thornton[2]; *Peter Voorhees*[1]; [1]Northwestern University; [2]University of Michigan

A combined theoretical and experimental approach is used to examine the nature of the coarsening process in morphologically and topologically complex two-phase microstructures found following dendritic solidification and in nanoporous gold. We examine the coarsening dynamics in three dimensions as a function of time using X-ray tomography and simulation. Using the two-point spatial correlations of the solid-liquid interfacial curvature, we show why dendritic solid-liquid mixtures exhibit classical $t^{1/3}$ kinetics for the average length scale, yet are not self-similar as theory predicts. Large-scale simulations of coarsening in bicontinuous mixtures under both surface or bulk diffusion have been performed to determine the interfacial shape distributions that can then be compared to the experimentally measured distributions to understand the nature of the coarsening process in these systems.

Energy Materials I

Monday PM
June 11, 2018

Room: Store Scene
Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

1:30 PM Invited

CINEMA - the allianCe for ImagiNg and Modelling of Energy Applications: *Jens Andreasen*[1]; Anders Dahl[1]; Henning Sørensen[2]; Lars Mikkelsen[1]; Erik Lauridsen[3]; Brian Vinter[2]; Carsten Gundlach[1]; Rajmund Mokso[4]; Henning Poulsen[1]; [1]Technical University of Denmark; [2]University of Copenhagen; [3]Xnovo Technologies; [4]MAX IV Laboratory

CINEMA is a strategic research alliance that focuses on development of in situ X-ray imaging and modelling of energy materials, with 15 PhDs and 5 post docs dedicated to the effort. The scope of CINEMA will be presented and an overview of the most important results, within development of in situ equipment for 3D imaging, and in analysis tools for quantification and modelling of 3D data. The tools developed are generic to most 3D imaging modalities and are disseminated to facilities such as MAXIV, through the Centre for quantification of imaging data from MAX IV (QIM), and to other fields, including electron imaging in a new European Innovative Training Network, MUMMERING. The methodology of 3D imaging, analysis and modelling is taught at an annual summer school CINEMAX, and through an interactive e-learning course eCINEMA, that will launch in 2018. Tools learned and applied in Jupyter notebooks will be demonstrated.

2:00 PM

High-resolution Mapping of Bismuth Ferrite-based Multiferroics by X-ray Diffraction Computed Tomography: *Marta Majkut*[1]; Hugh Simons[2]; Tadej Rojac[3]; Andreja Bencan Golob[3]; Jeppe Ormstrup[2]; John Daniels[4]; Jonathan Wright[1]; [1]European Synchrotron Radiation Facility; [2]Technical University of Denmark; [3]Jozef Stefan Institute; [4]University of New South Wales

Bismuth ferrite-based ceramics are multiferroics with interesting properties such as an electric-field-induced phase transformation that results in large macroscopic strain, thus making these materials attractive candidates for electromechanical applications. As in many polycrystalline materials, such macroscopic responses are highly influenced by grain-scale heterogeneities and intergranular interactions, and their study benefits from grain-resolved characterisation techniques such as three-dimensional X-ray diffraction (3DXRD). While 3DXRD has successfully been applied to coarse-grained materials, fine-grained materials such as bismuth-ferrite have proven challenging due to limited spatial resolution and a 'powder-like' diffraction pattern in which diffraction spots cannot be resolved. The nano-focus end-station at beamline ID11 at the ESRF offers a solution with an X-ray diffraction computed tomography approach using a ~200 nm x 200 nm focussed beam. We present the high-resolution grain map of a bismuth-ferrite ceramic highlighting microstructure and grain neighbourhood properties, and the impact on studies of other sub-micron scale materials and phenomena.

2:20 PM
Sulphur Evolution Before and After Cycling in Lithium-sulphur Batteries Revealed by High Resolution X-ray Tomography: *Shao-Gang Wang*[1]; Lei Zhang[1]; [1]Institute of Metal Research, Chinese Academy of Sciences

Li-S batteries are considered to be a promising next generation high energy electrochemical energy storage system. The specific capacity and energy density of Li-S batteries is strongly related to its sulphur loading (mg cm-2) and sulphur content (wt. %). Ingenious design of 3D electrode structures can simultaneously improve the sulphur loading and sulphur content while keep good electrochemical properties for high performance Li-S batteries. In this talk, four elaborate 3D electrode microstructures such as a 3D hybrid graphene hierarchical network macrostructure will be presented. Multi-scale in-situ and ex-situ ultra-high resolution lab-based 3D X-ray tomography techniques with the pixel size from 65 nm to 20 um were explored to reveal the 3D and 4D evolution characteristics of sulphur in these state-of-the art electrodes before and after cycling. Our results would lay insight on the design and development of high specific capacity, high specific energy density and long life Li-S batteries.

2:40 PM
3D Characterization of Nuclear Fuels by Neutron Diffraction and Energy-resolved Neutron Imaging: Kenneth McClellan[1]; Anton Tremsin[2]; Adrian Losko[1]; *Sven Vogel*[1]; [1]Los Alamos National Laboratory; [2]University of California Berkeley

3D characterization of nuclear fuels pre- and post-irradiation is of paramount importance to maximize the knowledge gain from expensive irradiation tests. Due to the heavy elements present in ceramic (U-O, U-Si, U-N, U-C etc.) or metallic (U-Mo, U-Pu-Zr etc.) fuels, X-ray and synchrotron characterization is limited to small volumes. At LANSCE, the unique advantages of neutrons for characterization of nuclear fuel materials are applied to accelerate the development of new nuclear fuel forms. By characterizing slices or volumes within the sample, spatially resolved measurements of phase composition, strains, and textures are possible. In parallel, energy-resolved neutron tomography is developed, not only allowing to visualize cracks, arrangement of fuel pellets in rodlets etc., but also characterization of isotope densities by means of neutron absorption resonance analysis. This novel approach allows spatial resolution below 50 micrometer. We provide an overview of characterizations for accident-tolerant fuel consisting of uranium nitride/uranium silicide composite fuels.

3:00 PM
Sample Design and Preparation Techniques for Dynamic Microstructural Studies of High Temperature Electrochemical Cells: *Jacob Bowen*[1]; Salvatore De Angelis[1]; José Xavier Trujillo; Peter Jørgensen; Esther Hsiao Rho Tsai[2]; Mirko Holler[2]; Julie Villanova; [1]Technical University of Denmark; [2]Paul Scherrer Institute

Understanding the dynamics of 3D microstructural change in high temperature electrochemical cells, primarily solid oxide fuel cells or electrolysers, is a pressing driving force for performing time resolved ex-situ, in-situ and in-operando nano-tomography and diffraction based experiments at synchrotron X-ray sources. These experiments must meet simultaneous challenging demands: precision beamline compatible samples that are stable at high temperature, supply of electric potential, and control of atmosphere. Correct sample design is an absolute necessity for experimental success. Here, the merits of possible sample configurations and environments are explored and evaluated against fabrication challenges and experimental feasibility. Experience with designing and performing experiments of selected configurations will be presented. Results of 3D nano-tomography of Ni-yttria stabilized zirconia (YSZ) fuel electrode microstructure evolution during Ni oxidation, reduction and annealing, and spatially resolved in-operando diffraction studies of YSZ electrolytes under at high polarization will be summarised.

3:20 PM Break

Porous and Nanostructured Materials I

Monday PM June 11, 2018	Room: Lille Scene Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

1:30 PM Invited
3D Grain Mapping of Open-cell Aluminum Foam by Synthetic-data Fusion with Experimental Data from HEDM: Jayden Plumb[1]; Jonathan Lind[2]; Joseph Tucker[3]; Ron Kelley[4]; *Ashley Spear*[1]; [1]University of Utah; [2]Lawrence Livermore National Laboratory; [3]Exponent Failure Analysis Associates; [4]Thermo Fisher Scientific

Open-cell metal foams are low-density, structural-material systems that derive their mechanical properties from a combination of their parent alloy and their structural topology and morphology. Recent work also suggests that grain structure could play a significant role in the local deformation behavior of individual ligaments, which could potentially translate across length scales. This talk describes recent efforts to map 3D grain structure in investment-cast, open-cell aluminum foam. Several advanced techniques have been integrated to digitally represent a physically-realized foam by both its geometry/topology as well as its underlying polycrystalline structure. Namely, experimental measurements were conducted using X-ray computed tomography and far-field high-energy X-ray diffraction microscopy (HEDM), and the experimental data were augmented using synthetic-grain instantiation within DREAM.3D. The grain-resolved mapping achieved by fusion of synthetic and experimental data marks a critical step toward investigating relationships among manufacturing/process parameters, microstructure, and mechanical behavior across multiple length scales in open-cell metal foams.

2:00 PM
In-situ Compression Testing of High-strength Low-weight Micro- and Nanolattices Using Nano-scale X-ray Imaging: Almut Schroer[1]; *Hrishikesh Bale*[2]; Jens Bauer[1]; Ruth Schwaiger[1]; [1]Karlsruhe Institute of Technology; [2]Carl Zeiss Microscopy Inc.

Significant advancements in the nanoscale direct-write two-photon lithography technique have enabled the fabrication of intricate hierarchical 3D structures, otherwise referred to as metamaterials. Furthermore, an overall improvement in strength nearing the theoretical strength of certain materials such as glassy carbon can be achieved through a combination of direct write and pyrolysis. The challenges, however, have remained in characterizing the 3D structures and understanding the failure mechanisms within these complex 3D nano-architectures. In-situ tests conducted in a scanning electron microscope provide only 2D surface information. 3D nanoscale X-ray tomography can provide valuable 3D information non-destructively at up to 16nm/voxel 3D resolution. We present here, results from an in-situ nano-scale compression test conducted on a 3D nano-lattice truss structure in a nanoscale x-ray microscope. 3D reconstructions clearly resolved individual truss members and were observed to deform with applied load. Results of strain analysis using digital volume correlation will also be discussed.

2:20 PM
A Multianalytical Approach towards a Comprehensive Characterization of Nanoporous Gold: *Markus Ziehmer*[1]; Kaixiong Hu[1]; Anton Davydok[1]; Jean-Sébastien Micha[2]; Imke Greving[1]; Emanuel Larsson[1]; Christoph Kirchlechner[3]; Erica Lilleodden[1]; [1]Helmholtz-Zentrum Geesthacht; [2]European Synchrotron Radiation Facility; [3]Max-Planck-Institut für Eisenforschung

Nanoscale materials naturally pose a challenge with respect to achieving a comprehensive microstructural characterization. This may be even more so the case for materials exhibiting an inherently complex appearance, like nanoporous gold (npg). Due to its bicontinuous network structure, best described as interconnected rings, 3D analyses are mandatory. In addition to morphological and topological characteristics, accessed by tomography methods, crystallographical domain sizes are also critical to understanding structure-property relations, necessitating diffraction techniques. Furthermore, the ability to thermally coarsen the network structure, i.e. the ligaments as well as the rings, impose another complexity factor. We present results from a multianalytical approach to determine and quantify the critical structural elements of npg along with their thermal evolution. This includes 3D FIB tomography, 3D X-ray nanotomography, X-ray microLaue diffraction, and EBSD. We highlight the importance of our findings in understanding the properties of npg, with a focus on mechanical properties.

2:40 PM
4D Granular Mechanics: Fabric, Strain and Force Transfer from In-situ X-ray Tomography and 3DXRD: *Stephen Hall*[1]; Ryan Hurley[2]; Eric Herbold[3]; Jonathan Wright[4]; Marta Majkut[4]; Jonas Engqvist[1]; [1]Division of Solid Mechnics, Lund University; [2]John Hopkins University; [3]Lawrence Livermore National Laboratory; [4]European Synchrotron Radiation Facility

A better understanding of deformation and failure in granular materials is key to many engineering applications. However, the mechanics of granular materials are complex, involving the deformation and interactions of many individual grains and the transfer of forces between them. Recent experimental advances, combining in-situ loading experiments, x-ray tomography and 3DXRD, have enabled new insights into granular mechanics. X-ray tomography provides details on granular structure and its evolution, including grain reorganization and breakage. 3DXRD can reveal the elastic deformation of the individual grains that, combined with the grain contacts from tomography, can be used to infer contact force networks through a granular assembly. Furthermore, with appropriate image analysis, continuum strain fields can be determined from the evolving grain centre-of-mass positions. We will describe these methods and their potential with new results revealing the coupling of heterogeneous deformation and evolving force networks in granular materials under different loading conditions.

3:00 PM
Dynamic X-ray Imaging in the Laboratory: *Arno Merkle*[1]; Marijn Boone[1]; Denis Van Loo[1]; [1]XRE

Time-resolved 3D imaging with X-rays has rapidly emerged as an essential technique to understand materials evolution, facilitating in situ investigations ranging from mechanical deformation to fluid flow in porous materials and beyond. Synchrotron radiation facilities have spearheaded this push toward time-resolved dynamic studies with quite some success. Meanwhile, in the laboratory where majority of the complementary parts of scientific investigations occur, X-ray imaging has steadily improved, approaching spatial resolutions achieved at many synchrotron facilities. However, these tremendous gains have often come at a significant cost of temporal resolution. Recently, developments at XRE have made it possible to explore dynamic processes in the laboratory, achieving tomographic temporal resolution below 10 seconds. Here we explore the innovations that have led to this capability, including hardware design optimization and significant software advances in acquisition, reconstruction and analysis. Details of these methods will be illustrated by way of a foam collapse study.

3:20 PM Break

Corrosion and Fracture I

Monday PM
June 11, 2018

Room: Lille Scene
Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

3:50 PM
4D Non-destructive Investigations of the Influence of Crystallographic Orientation and Microstructure on Corrosion in Aluminum Alloys: Tyler Stannard[1]; Sridhar Niverty[1]; Jacob Graber[1]; Jason Williams[1]; Hrishikesh Bale[2]; Nicolas Gueninchault[3]; *Nikhilesh Chawla*[1]; [1]Arizona State University; [2]Carl Zeiss Microscopy Inc.; [3]Xnovo Technology ApS

Aluminum alloys used extensively in aircraft components and skins are frequently exposed to harsh environments; corrosive saltwater spray combined with the fatigue stresses of flight operations in service. Several factors including the underlying microstructure, defects, and crystallographic grain orientation play a dominant role in corrosion-related fracture of these alloys. Grain mapping techniques like EBSD are restricted to 2D surface imaging and can only be extended in 3D through destructive sectioning. Laboratory-based diffraction contrast tomography (LabDCT) is possible on a commercially available X-ray microscope, enabling time-dependent '4D' corrosion studies, wherein samples can be imaged in 3D at high resolution to understand the complex mechanisms of corrosion. Here, we present experimental results acquired on aluminum 7475 using LabDCT that investigate corrosion behavior of these alloys. Further examination of the influence of inclusions, triple point grain boundaries and misorientation on the corrosion evolution based on the 3D data analysis will also be discussed.

4:10 PM
Understanding Environmentally Assisted Cracking of High Strength Aluminium Using In Situ X-ray CT: *Tim Burnett*[1]; Henry Holroyd[2]; John Lewandowski[3]; Malte Storm[4]; Philip Withers[1]; [1]University of Manchester; [2]Consultant; [3]Case Western Reserve University; [4]Diamond Light Source

Environmentally assisted cracking of high strength aluminium has been the subject of research effort for over 50 years and yet it is still poorly understood. Slow strain rate tests have been conducted in situ on high strength aluminium combined with synchrotron X-ray CT. The growth and morphology of the cracks has been investigated and quantified. The failed specimens were then studied using SEM fractography linking many aspects of the microstructure to the crack morphology. We will present the new insights into the initiation and propagation of these environmentally assisted cracks.

4:30 PM
Crack Morphology in a Columnar Thermal Barrier Coating System: *Anne Dennstedt*[1]; Fabrice Gaslain[1]; Marion Bartsch[2]; Vincent Guipont[1]; Vincent Maurel[1]; [1]Centre des Matériaux - Mines Paristech - CNRS UMR 7633; [2]German Aerospace Center (DLR)

Ceramic layers are used as thermal barrier coatings (TBCs) on metallic substrates. During thermal transients, the thermal expansion mismatch between coating and substrate drives failure of the TBC mainly by interfacial cracking. Laser Shock Adhesion Test (LASAT) provides stresses at the ceramic/metal interface enabling controlled interfacial cracking. For achieving a clear understanding of the influence of local morphology on interfacial toughness, this study aims at characterizing the 3D morphology of a crack at the interface between metal and an EB-PVD TBC having a columnar structure. Cracks were produced by LASAT and documented further in SE and BSE image stacks collected simultaneously during subsequent slice and view operations using a focus ion beam (FIB) and a scanning electron microscope (FIB slice & view). The segmented 3D data gives clear understanding of the columnar structure of the ceramic and of the interaction between the crack and the TBC microstructure.

4:50 PM
3D Characterisation of Iodine-induced Stress Corrosion Cracks in Zirconium Alloys: *Alistair Garner*[1]; Conor Gillen[1]; Philipp Frankel[1]; [1]University of Manchester

X-ray computed tomography is used to map the locations and morphology of iodine-induced stress corrosion cracks in zirconium alloys, generated by stressing C-ring samples in iodine-ethanol solution. The presence of iodine is identified using nanoscale secondary ion mass spectrometry and a crack tip region is lifted out for serial sectioning analysis using a Xe plasma focused ion beam (PFIB). Due to high milling rates in the PFIB, a relatively large volume can be analysed with complementary acquisition of both chemical and crystallographic information. The 3D orientation information is correlated to the 3D crack path reconstructed from electron images. Attacked grain boundaries (GBs) are identified from the aligned datasets, from which the GB plane is estimated by fitting a plane to the neighbouring grains surface mesh. This allows for a large number of I-SCC susceptible GBs to be fully characterised and leads to new insight into crack propagation mechanisms.

5:10 PM
Topological Characteristics of Three-dimensional Grain Boundary Networks and Their Influence on Stress Corrosion Crack Propagation: *Tingguang Liu*[1]; Shuang Xia[2]; Bangxin Zhou[2]; Yonghao Lu[1]; Tetsuo Shoji[3]; [1]University of Science and Technology Beijing; [2]Shanghai University; [3]Tohoku University

Microstructures of 316L stainless steel before and after grain boundary (GB) engineering have been studied by using serial sectioning coupled with EBSD mapping in terms of 3D characterization. The twin boundary arrangement in the conventional and GB engineered GB networks were investigated and compared. Additionally, an intergranular crack and the GB network along the crack in the conventional 316L after stress corrosion cracking (SCC) test in high-temperature water were investigated in 3D. It was found that the proportions of triple junctions with two twin boundaries and quadruple junctions with three twin boundaries have a considerable increase after GB engineering. The twin boundaries not only show a strong resistance to cracking, but they could also prevent their neighboring boundaries from cracking, as the cracking probability is lower for boundaries that have higher fraction of neighboring twin boundaries.

5:30 PM
Development of a Micro-single Edge Notched Tensile (Micro-SENT) Testing to Determine Toughness Using X-ray Synchrotron Tomography: *Yazid Madi*[1]; Loic Courtois[2]; Joseph Marae-Djouda[3]; Clement Soret[4]; Maxime Pellerin[5]; Jacques Besson[5]; [1]EPF-Ecole d'ingénieurs / Centre des Matériaux Mines ParisTech; [2]3Dmagination Ltd; [3]EPF Ecole d'ingénieur-e-s; [4]ENGIE Lab - CRIGEN; [5]Mines ParisTech, PSL Research University, MAT-Centre des Materiaux

The toughness of a ductile steel used in the pipeline industry is investigated using both standard Single Edge Notched Tensile (SENT) specimen and a developed micro-SENT specimen. Micro-SENT sample is tested using in-situ X-ray synchrotron-radiation computed tomography (SRCT). As a first step, the notch is electro-discharge machined, in order to analyse local mechanical behaviour and damage of the small specimen compared to the conventional one. The SRCT high resolution technique is used to provide clear images to analyse quantitatively the damage evolution during both crack initiation and crack propagation. Indeed, the crack advance is directly measured during propagation and a J-da resistance curve is determined. Digital Image Correlation and Finite Element Analysis are also used to analyse the strain fields around the crack tip.

5:50 PM
In-Situ Synchrotron X-ray Micro-tomography of Microstructure Evolution during Ceramic Matrix Composite Processing: *Natalie Larson*[1]; Harold Barnard[2]; Dilworth Parkinson[2]; Alastair MacDowell[2]; Charlene Cuellar[3]; Richard Sim[4]; Frank Zok[1]; [1]University of California, Santa Barbara; [2]Lawrence Berkeley National Laboratory; [3]University of California, San Diego; [4]University of California, Berkeley

In-situ synchrotron x-ray computed micro-tomography at the Advanced Light Source has been used to observe microstructure evolution during ceramic matrix composite processing. In one set of experiments, impregnation of a liquid matrix precursor into a fiber preform was imaged *in-situ*. The resulting 4D datasets (1µm^3 resolution, 1.5 min sequential scans) reveal fiber movement and void formation over time for a wide range of impregnation speeds. In another set of experiments, polymer-to-ceramic conversion of a preceramic polymer matrix in a SiC fiber preform was imaged *in-situ* at temperatures up to 1200°C. The resulting 4D datasets (1µm^3 resolution, 12 min sequential scans) reveal the spatial and temporal evolution of a complex hierarchy of shrinkage cracks. A quantitative assessment of the microstructure evolution during processing will be presented for both experiments. Additionally, recent developments in the techniques and instrumentation for these and future *in-situ* processing experiments will be discussed.

Dislocations, Twins, Strain, and Plastic Deformation I

Monday PM
June 11, 2018

Room: Store Scene
Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

3:50 PM Invited
Intra-granular Strain Sensitivity in Near-field High Energy Diffraction Microscopy: Yufeng Shen[1]; He Liu[1]; *Robert Suter*[1]; [1]Carnegie Mellon University

Near-field High Energy x-ray Diffraction Microscopy (nf-HEDM), a synchrotron-based, non-destructive, 3-D characterization technique, has been used to measure grain maps of various materials, from elemental metals to complex industrial alloys in states from pristine to significantly deformed (ex. 15% tensile extension). Voxel based forward modeling reconstructions demonstrate sensitivity to intra-grain orientation variations. Here, we demonstrate intra-grain elastic strain sensitivity based on the observation that, in some data sets, projected images of grains are split between different detector images; that is, strain states are distinguished through sensitivity to the sample rotation angle, omega, rather than through variations in scattering angle, two-theta. Such sensitivity offers unique opportunities for testing and developing theoretical and computational models of materials responses. This talk will discuss the level of strain sensitivity and the conditions under which this information can be extracted. Examples will include both simulated and experimental data.

4:20 PM
3D Dislocation Structures in Experiment and Modeling: *Gabor Ribarik*[1]; Gyula Zilahi[1]; Éva Ódor[1]; Tamás Ungár[1]; [1]Eotvos Lorand University

Dislocation structures are three dimensional (3D) and grain structures in polycrystalline materials are also 3D. There are two fundamental methods to determine the dislocation structure: Electron Microscopy (EM) and X-ray Line Profile Analysis (XLPA). EM gives visual and detailed information of the type of dislocations, however, the volume of inspection is often limited. XLPA provides larger averages and can provide better information about strains and stresses. X-ray powder diffraction, though a powerful method, gives averages over millions of grains which may be very different in the individual structures. Recent high angular resolution synchrotron experiments have been carried out on polycrystalline samples providing single crystal line profile analysis giving detailed information on Burgers vector population and dislocation densities in single grains of a large variety of materials. We shall discuss the basics of single grain XLPA in polycrystalline samples and attempt to correlate the experimental results with modeling by numerical simulations.

4:40 PM
Development of an In-situ Straining and Time-resolved Electron Tomography Data Acquisition System: *Satoshi Hata*[1]; Shinsuke Miyazaki[2]; Takeshi Gondo[3]; Katsumi Kawamoto[4]; Noritaka Horii[4]; Kazuhisa Sato[5]; Hiromitsu Furukawa[4]; Hiroyuki Kudo[6]; Hiroya Miyazaki[3]; Mitsuhiro Murayama[7]; [1]Kyushu University; [2]Thermo Fisher Scientific; [3]Mel-Build Corporation; [4]System in Frontier Inc.; [5]Osaka University; [6]University of Tsukuba & JST-ERATO; [7]Virginia Tech

We designed an integrated system using a straining-and-tomography specimen holder and newly developed software for specimen-straining and image-acquisition and then developed an experimental procedure for in-situ straining and time-resolved electron tomography (ET) data acquisition. The software for tilt-series dataset acquisition and 3D visualization was developed based on the commercially available ET software TEMography. We achieved time-resolved 3D visualization of nanometer-scale plastic deformation behavior in a Pb-Sn alloy sample, which demonstrates the capability of this system for potential applications in 3DMS.

5:00 PM
Insight into the Kinetics of Plasticity Using High-energy X-ray Diffraction: *Armand Beaudoin*[1]; Darren Pagan[1]; Kamalika Chatterjee[1]; Paul Shade[2]; Matthew Miller[1]; Sol Gruner[1]; Hugh Philipp[1]; Mark Tate[1]; [1]Cornell University; [2]Air Force Research Laboratory

Constitutive models for crystal plasticity are developed by relating a model idealization to (typically) scalar data from mechanical testing. High-Energy Diffraction Microscopy (HEDM), a technique using synchrotron radiation for study of polycrystalline materials, provides tensorial information that may be applied directly in validation of models for polycrystal plasticity. Advances in detector technology provide for extending the application of HEDM to details of the kinetics of plasticity. This is of particular consequence when multiple mechanisms of deformation are active – something quite difficult to sort out through traditional mechanical testing. In this work, we utilize a Mixed-Mode Pixel Array Detector with a CdTe sensor layer to explore transient plasticity in several different metals and alloys. Examples relating to the kinetics and intermittency of slip will be presented. Techniques of unsupervised learning will be applied in the analysis of diffraction data.

5:20 PM
3D Analysis of the In-grain Orientation Spreads in Deformed Aluminium by 3DXRD-based Measurements and Finite Element Simulations: *Romain Quey*[1]; Loïc Renversade[1]; [1]Mines Saint-Etienne

The development of the orientation distributions of 500 grains of an aluminium polycrystal deformed in tension were analysed. The undeformed microstructure was first characterized using diffraction contrast tomography (DCT). The grain lattice rotations were then followed by 3D X-ray diffraction microscopy (3DXRD) up to a strain of 4.5%. A new method was developed to extract the in-grain orientation distributions from the diffraction peaks, in which the parameters of a model orientation distribution are determined using forward simulation of diffraction and optimization. The properties of the orientation distributions were then analysed in terms of angular extent and anisotropy. It is shown that the 1st principal axes preferentially align with the tensile direction at strain lower than 2% and then migrate to a direction normal to the tensile direction. The results were compared to a crystal plasticity finite element simulation, and an agreement was concluded at largest strains.

5:40 PM
Single Grain High Resolution Reciprocal Space Mapping: *Ulrich Lienert*[1]; Christian Wejdemann[2]; Wolfgang Pantleon[3]; [1]Deutsches Elektronen-Synchrotron; [2]Roskilde Katedralskole; [3]Technical University of Denmark

In-situ structural characterization on the subgrain length scale within polycrystalline bulk materials has been demonstrated exploiting the high brightness of 3rd generation high-energy synchrotron facilities. At PETRA III the Swedish materials science beamline has been constructed and is expected to see first light in 2018. The capabilities regarding to 3D characterization will be described with particular emphasize on high resolution reciprocal space mapping (HRRSM). Dramatic further improvements will result from ongoing storage ring upgrades and efficient (CdTe) pixel detectors.The potential of HRRSM will be illustrated by a case study investigating strain path changes in copper. A statistically significant number of subgrains was identified. The existence of a microplastic regime was revealed during which only the subgrains deform plastically and no yielding of the dislocation walls occurs. Second, after reloading above 0.3% strain, the elastic stresses of individual subgrains are about the same as in uni-directionally deformed reference specimens.

6:00 PM
Strain Field Around a Tin Whisker Studied Using Differential Aperture X-ray Microscopy (DAXM): *Johan Hektor*[1]; Jean-Baptiste Marijon[2]; Matti Ristinmaa[1]; Stephen Hall[1]; Håkan Hallberg[1]; Srinivasan Iyengar[1]; Jean-Sébastien Micha[3]; Odile Robach[3]; Fanny Grennerat[4]; Olivier Castelnau[2]; [1]Lund University; [2]Laboratory PiMM, Paris; [3]BM32, ESRF; [4]LGT Argouges

Tin (Sn) whiskers are microscopic, hair-like, grains that grow spontaneously out of surfaces coated with tin. Short circuits due to whisker growth have caused failure of many electronic components such as satellites, pacemakers and cell phones. It is generally accepted that whisker growth is a stress relaxation phenomena driven by strain gradients in the tin coating. However, experimental studies of the strain field around tin whiskers is largely missing. We have used Differential Aperture X-ray Microscopy (DAXM) to reconstruct the microstructure and strain field around a growing tin whisker in 3D. It was found that the deviatoric strain is high deep in the coating, where stress is generated due to formation of intermetallic compounds, and lower close to the whisker. Furthermore, there is a gradient in volumetric strain away from the whisker. This strain gradient is consistent with the expected driving mechanism for whisker growth.

Tuesday Plenary

Tuesday AM	Room: Store Scene
June 12, 2018	Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

8:00 AM Plenary
Polycrystalline Materials in 4 Dimensions: *Henry Proudhon*[1]; [1]MINES ParisTech

Non-destructive synchrotron 3D microstructural imaging is now mature and can be paired with mechanical loading (4D testing) and subsequent mechanical simulations at the grain scale. This is a key to advance our understanding of how the polycrystalline microstructure controls the mechanical properties of structural materials. In the last years, large efforts were devoted to develop 3D orientation mapping capabilities in mm sized specimens, with micrometer spatial resolution. Automated serial sectioning methods paired with EBSD 3D orientation mapping, can target very complex microstructures although at the price of destructing the specimen. In parallel, the increasing popularity and capabilities of hard X-ray tomography coupled to diffraction to image the bulk of materials in three dimensions brings forward a new way to conduct microstructurally informed mechanical testing. In particular, Diffraction Contrast Tomography now provides 3D grain maps non destructively and allow further crystallographic specific investigations during mechanical testing. One of the key challenges is then to link 3D microstructure characterization tools with computational models (eg by finite elements or FFT) to predict engineering properties such as strength or fatigue resistance. In this presentation, examples of 3D experimental microstructure based large-scale computations using the crystal plasticity finite element method will be presented and compared with in situ mechanical testing experiments. Examples with microstructures obtained with both serial sectioning and Diffraction Contrast Tomography will be targeted. Simultaneous modeling/experimental approaches will be discussed in light of the results. One recurring difficulty in the field of 4D studies is the very small number of tested samples, due to the limit of synchrotron beam time availability and to the inherent difficulty to manipulate 4D data sets. Possible solutions to these problems will be discussed.

8:45 AM Question and Answer Period

9:00 AM Break

Dislocations, Twins, Strain, and Plastic Deformation II

Tuesday AM
June 12, 2018

Room: Lille Scene
Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

9:10 AM Invited
On the Distributions of Thermoelastic Fields Inside Three-dimensional Polycrystals: A Simulation Study: *Sukbin Lee*[1]; Myeongjin Lee; Youngkyun Son; Sihwa Sung; Gaeun Son; [1]Ulsan National Institute of Science and Technology

In this study, we first predict the distributions of elastic fields inside digitally generated threedimensional polycrystals using thermoelastic simulations. Then, the effect of 1) simulation boundary conditions, 2) mesh types, 3) grain boundary curvatures, and 4) thermoelastic simulation methods (i.e., finite element method vs. fast Fourier transform based method) on the distribution of thermoelastic fields is investigated. Especially, an extreme value analysis is adopted to analyze the hotspots inside the polycrystals, predicted from thermoelastic simulations. By performing so, one can qualify or quantify the effect of various conditions of both simulations and microstructures on the distribution of thermoelastic fields, leading to more accurate interpretation of the predicted fields and better expectation of the materials behavior under the applied conditions.

9:40 AM
The Effect of Helium Implantation on the Deformation Behaviour of Tungsten: X-ray Micro-diffraction & Crystal-plasticity: *Suchandrima Das*[1]; Edmund Tarleton[1]; David Armstrong[1]; Yevhen Zayachuk[1]; Wenjun Liu[2]; Ruqing Xu[2]; Felix Hofmann[1]; [1]University of Oxford; [2]Argonne National Laboratory

Tungsten is a primary candidate material for plasma-facing armour components in future fusion reactors. Fusion neutron bombardment produces defects in tungsten. Interaction of helium, which is produced by transmutation and also injected from the plasma, with these defects modifies their retention and behaviour. Here we examine the effect of helium-implantation-induced damage on deformation behaviour by comparing spherical nano-indents in unimplanted and helium-implanted regions of the same tungsten single crystal. Helium-implantation increases hardness and causes large pileups. 3D-resolved X-ray micro-diffraction uniquely allows investigation of the complex lattice distortions beneath indents. Ion-implanted material shows reduced lattice rotations and residual strains due to indentation, indicating a more confined plastic zone. These observations suggest that initially helium-induced defects obstructs dislocation motion, but are weakened by the subsequent passage of dislocations, leading to reduced work hardening capacity. Initial progress with capturing these effects using 3D crystal plasticity finite element calculations is presented.

10:00 AM Break

10:30 AM
Development of Three-dimensional Inhomogeneous Plastic Strain during Cold Rolling in Al-Mg Alloys: *Masakazu Kobayashi*[1]; Tomoya Aoba[1]; Hiromi Miura[1]; [1]Toyohashi University of Technology

To understand local inhomogeneous deformation during thermo-mechanical processing is very important for understanding and prediction of microstructure development, because localized deformation would be one of key mechanism to control recrystallized texture. In this study, development of inhomogeneous plastic strain in three-dimension had been measured in cold rolled Al-Mg alloys that contain small lead particles, which are marker of local strain measurement, by using synchrotron radiation micro-tomography at BL20XU in Japanese synchrotron radiation facility, SPring-8. After synchrotron radiation experiment, the obtained tomographic images were image processed and analyzed to reproduce three-dimensional plastic strain maps. The strain distributions in different Mg content and rolling ratio were compared with microstructures obtained by SEM/EBSD. The relationship between local deformation evolution and grain microstructure is discussed.

10:50 AM
Intragranular Orientation Spread in Tensile-deformed Grains in Austenitic Steel: *Nicolai Juul*[1]; Jette Oddershede[2]; Grethe Winther[1]; [1]Technical University of Denmark; [2]Xnovotech

A 0.7x0.7x0.5 mm3 volume of a 316L austenitic stainless steel sample was examined by 3DXRD at CHESS. The sample was subjected to tensile deformation while illuminated during several load steps, resulting in a successful characterisation of the tensile-deformation behaviour of more than 300 grains up to 5% elongation. The focus is on the introduced intragranular orientation spread (mosaicity) of individual grains representatively chosen from the data set. Initially, the volume was illuminated in a near-field detector setup, ensuring an accurate spatial map of the undeformed microstructure, which serves as an ideal input for a simulation of the experiment using the crystal plasticity finite element method. The simulation was analysed and reconstructed in a similar fashion to the experiment, using artificial diffraction software, to analyse the level of agreement with the measured mosaicity. This gives insight into the slip activity of the grains and the governing parameters of the simulated grains.

11:10 AM
Combining In-situ High-energy X-ray Diffraction Measurements with Finite Element Modeling: *Darren Pagan*[1]; Paul Shade[2]; Joel Bernier[3]; Armand Beaudoin[1]; Matthew Miller[4]; [1]Cornell High Energy Synchrotron Source; [2]Air Force Research Laboratory, Wright Patterson Air Force Base; [3]Lawrence Livermore National Laboratory; [4]Sibley School of Mechanical and Aerospace Engineering, Cornell University

As the use of high-energy diffraction microscopy methods increases, new ways to interface these data with computational models are also becoming increasingly wide spread. The ONR-sponsored In-Situ (Integrated Simulation and X-ray Interrogation Tools and training for micromechanics) center at the Cornell High Energy Synchrotron Source (CHESS) seeks to further bridge experimentally gathered diffraction data and computational models. In this presentation, the results from two projects combining diffraction experiments and modeling will be discussed. In the first, average grain stresses measured in-situ from a Ti-7Al specimen are used to develop and calibrate a new constitutive model that is evaluated using finite element crystal plasticity. The second project combines peak evolution data measured using the very-far field diffraction technique as a copper single crystal deformed in-situ with field dislocation mechanics to understand the stress distributions that develop during the formation of shear bands.

11:30 AM
Assessing Experimental Parameter Space for Achieving Quantitative Electron Tomography for Nanometer-scale Plastic Deformation: *Ya-Peng Yu*[1]; Joshua Stuckner[1]; Chang-Yu Hung[1]; Hiromitsu Furukawa[2]; Mitsuhiro Murayama[1]; [1]Virginia Tech; [2]System In Frontier, Inc

Integrating in-situ deformation and electron tomography techniques allows us to visualize the materials' response to an applied stress in three-dimension with nanometer scale spatial resolution and reducing several well-known artifacts such as the projection effect. On the other hand, implementing deformation mechanism introduces additional experimental constraints, for example, narrower tilt angle range, those could influence the accuracy of three-dimensional reconstruction in a different way. To materialize quantitative and statistically relevant microstructure interpretation by this technique, we evaluated several key parameters and their combinations to characterize their influences on the accuracy of size and morphology reproducibility. Observing morphology changes of nanostructured materials (a nanoporous gold) and defect structure representation in bulk materials were attempted as a model study.

11:50 AM
Individual Grains Behaviour during Superelastic Tensile Test of a Shape Memory Alloy Using 3DXRD Synchrotron Techniques and Diffraction Contrast Tomography (DCT): *Younes El-Hachi*[1]; Benoît Malard[2]; Sophie Berveiller[1]; Jonathan Wright[3]; Wolfgang Ludwig[3]; [1]Arts et Métiers ParisTech, LEM3; [2]CIRIMAT/ENSIACET; [3]ESRF

In superelasticity, the stress-induced transformation from austenite into martensite is observed in shape memory alloy; to predict it, the knowledge of the austenite stress state is required. The austenite stress state depends on its orientation, its grains size, and neighboring grains that induce intergranular stress interactions in the case of polycrystals. In order to better understand the contribution of each factor, two synchrotron techniques have been used to determine the mechanical behavior of hundreds of individual grains of a Cu-Al-Be polycrystal: the DCT gives access to the real 3D microstructure while the strain and stress tensors were determined by the 3DXRD technique. By DCT, the microstructure of the polycrystal was reconstructed. Correlations with 3DXRD results show that grains exhibit quite large stress depending on their orientation, but also their neighboring grains and their position in the specimen. Results are compared and discussed considering all these parameters.

Phase Transformations, Particle Coarsening, Grain Growth, and Recrystallization II

Tuesday AM
June 12, 2018

Room: Store Scene
Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

9:10 AM Invited
Toward High-throughput 3D X-ray Characterization: *Branden Kappes*[1]; Henry Geerlings[1]; Nathan Johnson[1]; Dana Drake[1]; Thomas Gallmeyer[1]; Aaron Stebner[1]; [1]Colorado School of Mines

High flux X-ray sources are making 3D characterization more accessible. While they enable characterization of microstructural, morphological and dynamical processes, these techniques produce large data sets; and large data sets impose both practical and analytical challenges. Working with information about many hundreds to thousands of grains fosters the need to develop techniques that can differentiate statistically averaged behavior from the effects of even isolated defects. For example, void formation at hard-soft grain boundaries, which would be hidden in texture analysis, is critical for the mechanical performance of additively manufactured titanium. In additive manufacturing, each machine-material combination requires new process conditions, so non-destructive testing is critical to correlate process parameters, microstructure and mechanical performance. This presentation will focus on the microstructure and morphology of additively manufactured Inconel 718 and Ti-6Al-4V and the data management, analysis and informatics challenges and solutions developed to identify trends across hundreds of X-ray data sets.

9:40 AM
In-situ 3DXRD Characterization of the Martensite Band Front in NiTi SMA Loaded in Tension: *Pavel Sedmak*[1]; Petr Sittner[2]; Jon Wright[1]; [1]ESRF; [2]Institute of Physics, ASCR

It has been known for a long time that the martensitic transformation in NiTi-based SMAs deformed in tension occurs by propagation of macroscopic martensite band fronts leading to plateau-type stress-strain curve. The mechanism, shape and the strain-stress state at the front were, however, unknown. We performed a dedicated 3DXRD experiment at the ID11 beamline to study the burried interface. Strain and stress tensors within ~15000 austenitic grains were determined. It was found that the interface has a conical shape and the strain-stress distribution at the interface is very inhomogeneous. A mesoscale mechanism of the localized deformation was revealed and described by thermomechanical FE model. Strains and stresses within the martensitic part of the wire were measured by x-ray diffraction tomography technique at the new ID11 nanostage and are confronted with the thermomechanical model.

10:00 AM Break

10:30 AM
Processing-microstructure Relationships in Isolated Melt Pools of Electron Beam Melted Inconel 718: *Andrew Polonsky*[1]; Narendran Raghavan[2]; McLean Echlin[1]; Michael Kirka[2]; Ryan Dehoff[2]; Tresa Pollock[1]; [1]University of California, Santa Barbara; [2]Oak Ridge National Laboratory

Recent advances in additive manufacturing (AM) techniques offer a vast design space to create optimized structures for a variety of applications, including the aerospace and medical industries. The interplay between processing conditions and ultimate performance of additive parts remains an area of intense study. In order to achieve improved functionality of components through novel design, a thorough understanding of microstructural development and solidification processes arising at the scale of the melt pool size is required. Structural and crystallographic information of isolated melt pools on the order of a cubic millimeter was collected in three dimensions using the TriBeam tomography system. By varying build parameters, morphologically distinct microstructures were created to determine the effects of preexisting microstructures on subsequent solidification events. A comparison between experimentally observed microstructures and theoretical predictions will also be presented.

10:50 AM
In Situ Hard X-ray Transmission Microscopy – Towards Space and Time Resolved Studies of Processes at the Nanoscale in Materials: *Ragnvald Mathiesen*[1]; Ken Falch[1]; Carsten Detlefs[2]; Marco Di Michiel[2]; Irina Snigireva[2]; Anatoly Snigirev[3]; [1]Norwegian University of Science and Technology; [2]ESRF; [3]Fed. Balt. Univ. Kaliningrad

Hard X-ray transmission microscopes are emerging at the new low-emittance synchrotron radiation sources. These instruments could pave the way for time-resolved in situ studies of microstructure formation and evolution at length scales down to 20-50 nm under realistic processing conditions. The new instruments could open for studies of several phenomena which in the past have been inaccessible via imaging-based approaches, such as self-organisation and pattern formation in nanomaterials, or heterogeneous nucleation processes. Access to experimental data at these time- and length scales would be of unprecedented value in the efforts to establish links between atomistic scale and continuum based computational models. The presentation will demonstrate various bright-field modalities of the instrument illustrated with a selection of possible case studies in material science.

11:10 AM
Reconstruction of Three-dimensional Ferrite–Austenite Microstructure and Boundary Migration Analysis in an Early Stage of Ferrite to Austenite Phase Transformation in Fe-Mn-low C Alloy: *Kengo Hata*[1]; Kaori Kawano[1]; Masaaki Sugiyama[2]; Tomoyuki Kakeshita[2]; [1]Nippon Steel & Sumitomo Metal corporation; [2]Osaka University

The crystallographic orientation relationship between ferrite and austenite in an early stage of the phase transformation upon heating has been investigated by three-dimensional EBSD analysis with FIB serial sectioning technique in Fe-Mn-low C steels. The three-dimensional ferrite–austenite microstructure was reconstructed from a microstructure quenched from the early stage of the phase transformation by determining the prior austenite orientation of the quenched martensite using a variant analysis method based on the K–S relationship. It was made clear that most of the austenite grains are transformed at grain corners in ferrite matrix. The crystallographic analysis has also revealed that the transformed austenite grain holds the K–S relationship or those close to it with two or three adjacent ferrite grains. Under in situ heating EBSD analysis on grain growth of the austenite at 790°C, the migration of the interfaces holding the K-S relationship is restricted.

11:30 AM
Characterising Microstructural Evolutions in Ice Cream Using Synchrotron X-ray Tomography: *Jingyi Mo*[1]; Enyu Guo[1]; Gerard Van Dalen[2]; Peter Schuetz[2]; Peter Rockett[1]; Peter Lee[1]; [1]University of Manchester - The Manchester X-Ray Imaging Facility; [2]Unilever R&D

Ice cream is a complex multi-phase colloidal system and its microstructure plays a critical role in determining consumers' taste experience. Prior studies on ice cream, using 2D cryo-SEM or ex situ tomography, provides limited insights into the dynamic processes and mechanisms. Here, we performed in situ in-line phase contrast synchrotron tomographic imaging on ice cream samples. A bespoke cold-stage capable of precise thermal control was used to cycle samples from 250 K to 267 K at two cooling rates of 0.05 k/min and 5 k/min while the samples being continuously tomographically imaged. The morphology of ice crystals during these dynamic cycles was quantified. Our results demonstrate the effect of temperature and time on the coarsening kinetics of both ice crystals and bubbles in ice cream. The microstructural evolution of this multi-phase material will also provide insight into other research domains e.g. freeze casting (ice templating) of novel bio-inspired scaffolding materials.

11:50 AM
New Possibilities Using Full Field High-tesolution 3D Synchrotron X-rays Methods for In-situ Recrystallization Studies: *Yubin Zhang*[1]; Dorte Juul Jensen[1]; [1]Technical University of Denmark

After 20-years development, the current generation synchrotron techniques, such as 3D X-ray Laue microdiffraction using differential aperture and diffraction contrast tomography, are powerful techniques for measurement of the crystallographic orientations, morphologies and local lattice strains of grains within bulk samples in full 3D. However, it is still challenging to study recrystallization of deformed metals with these techniques. In this presentation, several well-designed experiments performed using these techniques to study the recrystallization, including nucleation at hardness indents, grain boundary migration, and growth of several nuclei into a well-characterized deformation matrix will be presented. It is shown that with high-resolution (~1µm) mapping of both the deformation matrix and the recrystallized grains, the local heterogeneous nucleation and growth of recrystallized grains can be correlated to the local deformation microstructure. Key results are presented and it is discussed how the new results may be incorporated in next generation recrystallization models.

Energy Materials II

Tuesday PM June 12, 2018	Room: Store Scene Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

1:30 PM Invited
Phase-field Modeling on 3D Microstructure in Li-ion Battery Electrodes: *Baixiang Xu*[1]; Ying Zhao[2]; Peter Stein[1]; [1]Tu Darmstadt; [2]Cambridge University

Li-ion batteries are currently the most important energy storage technology. For both the functionality and the performance improvement, physical or designed spatially complex microstructure plays a critical role. For instance, new electrode materials involve phase separation during (de-)lithiation. Compared with dilute solution case, phase separation enhances heterogeneity and thus leads to harsher mechanical situation, which was deemed as one of the major degradation mechanisms of the battery. The composite structure of electrodes has also large impact on the effective conductivity of electrolyte, the electrochemical reaction and mechanical stability. Employing a multiphysics phase field theory and advanced 3D finite element simulations, we investigate the electrochemical and mechanical behavior of electrode particles during (de-)lithiation. Simulations demonstrate that phase separation results in an intensifed stress field and enhanced electrochemical reaction and even the crack propagation. Extensive simulations are carried out to explore the factors that contribute to the phase separation and battery performance.

2:00 PM
Time-resolved Neutron Radiography and Tomography of Red-ox Cycled Electrodes for Solid Oxide Electrochemical Cells: *Luise Kuhn*[1]; Malgorzata Makowska[2]; Monica Lacatusu[1]; Salvatore De Angelis[1]; Henrik Frandsen[1]; Erik Lauridsen[3]; Ingo Manke[4]; Manuel Morgano[5]; Markus Strobl[5]; Nikolay Kardjilov[4]; [1]Technical University of Denmark; [2]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II); [3]Xnovo Technology Aps; [4]Helmholtz-Zentrum Berlin fur Materialien und Energie; [5]Paul Scherrer Institute

We are reporting a combined study by time-resolved neutron radiography and tomography of red-ox cycling of electrodes for solid oxide electrochemical cells to analyze the degree of reduction/oxidation and e.g. crack formation. NiO/Ni-8YSZ (nickel/nickel oxide – yttria stabilized zirconia) are often used as electrodes in solid oxide electrochemical cells for efficient energy conversion (power-to-gas and vice versa) purposes. Results of in-situ 2D and ex-situ 3D measurements are presented. In-situ observation of phase transition between NiO and Ni were performed at BOA at the continuous neutron source SINQ at the Paul Scherrer Institute by monochromatic neutron imaging, and post mortem monochromatic neutron tomography was performed at CONRAD-2 at Helmholtz Zentrum Berlin at the BER II reactor. Combining both time resolved radiography and post mortem tomography, provides complementary information about the rate of chemical reactions and spatial evolution of phases and morphological changes, e.g. crack formation and thereby degradation of the electrodes.

2:20 PM
A Modelling Investigation of Solid Oxide Cells Degradation Based on Synchrotron X-ray Nanotomography Characterization: *Maxime Hubert*[1]; Jerome Laurencin[2]; Florence Lefebvre-Joud[2]; Peter Cloetens[1]; [1]European Synchrotron Radiation Facility; [2]CEA

The degradation of Solid Oxide Cells operating at high temperature is detrimental to consider their industrial deployment on a large scale. An approach based on electrochemical tests, advanced post-mortem characterization and multi-scale models has been used to investigate the link between the performances, the electrodes microstructure and their degradation upon operation. X-ray holographic nanotomography has been optimised at the ESRF to improve the spatial resolution and become virtually free of artefacts. It allows extracting the slow microstructural evolution in the Ni-YSZ hydrogen electrode. A physically-based model for Nickel agglomeration has been adjusted on the analysis performed on the 3D volumes and implemented in an in-house multi-scale modelling framework. The model has been used to quantify the contribution of Nickel agglomeration on the total degradation measured experimentally.

2:40 PM
3D Modelling of Ferroelectric Composite Properties using X-ray Micro Tomography Images: Effective Permittivity and Tunability: *Dominique Bernard*[1]; Catherine Elissalde[1]; Claude Estournes[2]; Julien Lesseur[3]; Erwan Plougonven[4]; Mario Maglione[1]; [1]ICMCB-CNRS; [2]CIRIMAT; [3]RXSolutions; [4]University of Liège

Ferroelectric materials are widely used in microelectronics and different approaches are explored to produce new materials. In the composite approach, dielectric particles are introduced in a ferroelectric powder to obtain by SPS a composite with dielectric inclusions distributed within a ferroelectric matrix. This presentation focussed on the final step where, for the same sample, measured and computed permittivities can be compared. We first exposed the numerical problem at the scale characterised by XCMT. Then, it is shown that the model reproduces the permittivity anisotropy induced by the deformation of the dielectric inclusions due to SPS. For tunability (permittivity variation with the applied electric field), Johnson's law is used as constitutive law and the dimensionless problem puts into evidence the main parameters. Fitting numerical and experimental results, this law allows reproducing the experimental data with precision, but requiring the introduction of an anisotropic non-linear coefficient. Consequences of this result are discussed.

3:00 PM Break

Porous and Nanostructured Materials II

Tuesday PM
June 12, 2018

Room: Lille Scene
Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

1:30 PM Invited
Correlating 3D Structural Characteristics to Micro-mechanical Behavior of Nanoporous Gold: *Erica Lilleodden*[1]; Kaixiong Hu; Markus Ziehmer; [1]Helmholtz-Zentrum Geesthacht

The mechanical behavior of NPG has been shown to be strongly dependent on its average ligament width, with local stresses approaching the theoretical strength of gold, underscoring the "smaller is stronger" paradigm. Such size-dependent strength can be exploited in NPG through targeted annealing in order to tailor the structural length-scales. Yet strong deviations from classical laws for cellular structures have been found for NPG, pointing to the need for developing new scaling laws for the prediction of mechanical properties as a function of structural length. This in turn is reliant on a more detailed investigation of the 3D network structure and crystallographic domain sizes, and a better understanding of the underlying structure-property relations governing mechanical response. By employing a combination of high-resolution tomographic characterization, micro-Laue diffraction and in situ micromechanical testing, the structure-property relations and mechanisms of deformation of this NPG have been explored and quantified. Using focused ion beam (FIB) based tomography applied to as-dealloyed and isothermally annealed NPG samples, we show that the ligament width distributions coarsen in a sufficiently self-similar, time-invariant manner, while the scaled connectivity density shows a self-similar ligament network topology, best described as a load-bearing ring structure. Such a ring structure has been quantified through an analysis of the mean principal curvatures, results from which are correlated to observations from in situ micromechanical experiments showing that the ring structure – rather than the solid volume fraction – governs structural stiffness.

2:20 PM
Quantifying Enhanced Oil Recovery in Synthetic Media with MicroCT: *Sidnei Paciornik*[1]; Kamila Scheffer[1]; Marcio Carvalho[1]; Yves Méheust[2]; [1]PUC-Rio; [2]Université Rennes 1

Enhanced oil recovery methods are tested and optimized in synthetic media, emulating porosity and permeability of real oil-bearing rocks. Such a medium was produced with sintered bi-disperse glass beads and microCT images (4 µm resolution) were acquired at different stages of fluid motion through the medium. Synthetic seawater with or without oil/water emulsion was used to recover oil previously saturating the medium´s pores. The water was doped with KI to fine tune X-ray absorption. Thus, 3D images showing the beads, doped water and residual oil presented a 3-modal histogram. After denoising with a non-local means filter, the images were segmented and the distribution of residual oil ganglia was visualized and quantified. Probability density functions of volumes (~10^4 ganglia spanning 8 orders of magnitude) show well defined exponential behaviors for the displacement of oil by water, while the use of emulsions provides better recovery efficiency with larger numbers of larger ganglia.

2:00 PM
Analysis of Cone Penetration Tests in Snow with X-tay Tomography: *Isabel Peinke*[1]; P. Hagenmuller[1]; E. Ando[2]; F. Flin[1]; G. Chambon[3]; J. Roulle[1]; [1]Météo-France - CNRS; [2]UGA, CNRS; [3]UGA, Irstea

Cone penetration tests (CPT) are common to get vertical profiles of snow hardness. To link the measured penetration strength, especially its high-frequency fluctuations, to microstructural snow characteristics such as grain size or density, it is necessary to understand the processes occurring next to the cone tip. Indeed, the snow closed to the cone tip gets compacted during the indentation, which affects the strength measurements. To decipher this link, we combined 3D micro-tomography imaging of snow and highly-resolved CPTs. Several samples spanning different snow types were imaged twice at a resolution of 15 microns: once before and once after a CPT. We developed an algorithm to fully recover and quantify the displacements between the pre-CPT and post-CPT images, which is a difficult task due to the presence of very large discontinuous displacements. The method combines image correlation and grain matching based on morphological criteria. The 3D displacement field will give us information of the re-organization of the bonds and thus new insights to interpret CPT in terms of microstructural characteristics.

2:40 PM
X-ray CT Based 3D Characterization of Closed-cell Aluminium Foams to Explore the Structure-property Relationship during Impact: *Mohammad Saadatfar*[1]; Abdul Kader[2]; [1]Australian National University; [2]University of New South Wales

Closed-cell aluminium foams are mostly used to mitigate the impact and blast load in order to safe products and personnel. The mechanical properties including the impact energy absorption capacity of foams are the direct consequences of their topological/geometrical collapse mechanisms during impact. In the present study, interrupted drop-weight impact experiments have been conducted to investigate the deformation evolution/collapse mechanisms of closed-cell aluminium foams. The sample has been compressed with total 21 interrupted drop impacts at strain rate ~ 40 s-1 and the post impacted samples have been imaged at four different strain states with high-resolution x-ray computed tomography. Our results show that the deforming microstructure creates strong correlations across a range of geometrical and shape characteristics. Further, we show that the deformation mechanism leaves topological signatures in the evolving microstructure, which can be used to better understand the mechanical response of the specimen at various stages of impact-deformation.

3:00 PM
Stress Test of a PVC Sample – DVC and Pore Network Modeling Analysis: *Cornelia Vacar*[1]; [1]Thermofisher Scientific

This study analyzes the effect of applying an increasing pressure on a PVC sample. The deformation of the sample through time is studied as it extends due to applying increasing amounts of load. Once a critical amount of load is reached, the material tears. By looking at the structure of the material (porous plastic) we can anticipate based on the pore density, the pore size and throat size where the tear is more likely to appear. Moreover, by applying a Digital Volume Correlation analysis and studying how the forces are distributed in the volume, we investigate a potential relation between the Pore Network Model of the material and the stress distribution in the volume. The PNM and the DVC are computed using the Avizo software and the data is provided by Shimadzu Techno-Research, Inc.

3:20 PM Break

Dislocations, Twins, Strain, and Plastic Deformation III

Tuesday PM
June 12, 2018

Room: Store Scene
Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

3:50 PM Invited
The Role of Atom Probe Tomography on the Development of the Next Generation of High Performance Materials: *Paraskevas Kontis*[1]; Surendra Makineni[1]; Leigh Stephenson[1]; Yanhong Chang[1]; Jonathan Cormier[2]; Dirk Ponge[1]; Dierk Raabe[1]; Baptiste Gault[1]; [1]Max-Planck-Institut für Eisenforschung GmbH; [2]Institut Pprime

Understanding the deformation mechanisms observed in high performance materials allows to design strategies for the development of materials exhibiting enhanced performance. New insights into these mechanisms can now be gained through systematic, high-resolution characterisation, enabled by advanced characterisation methods that offer spatially resolved quantification of deformation, on the one hand, and composition on the other. We base our work on the combination of structural information gained from electron microscopy and compositional measurements from atom probe tomography (APT). Regarding the latter, recent instrumentation developments also allow us to investigate challenging mechanisms such as hydrogen embrittlement. The impact of APT on the interpretation of deformation mechanisms in superalloys and titanium alloys will be presented.

4:20 PM
3D Reconstruction of The Spatial Distribution of Dislocation Loops with Least Square Fitting Approach: *Hongbing Yu*[1]; Xiaoou Yi[2]; Felix Hofmann[1]; [1]University of Oxford; [2]University of Science and Technology Beijing

We propose a new approach for reconstructing the 3D spatial distribution of small dislocation loops (DLs). It is based on fitting of specific DLs in multiple weak-beam dark field TEM micrographs recorded at different tilt angles. Each DL is identified in all the projections where it appears using a forward prediction approach. A system of linear equations can then be setup, linking the 3D position of each DL to its 2D position in each projection. If more than 2 projections are available, this system of equations is over-determined and the 3D position of each DL is found by least square fitting. This approach is applied to the damage formed by low-dose self-ion implantation in tungsten. The results are in good agreement with the damage microstructure recovered using a generalized weighted back-projection method. The advantages of the new triangulation approach are discussed in detail.

4:40 PM
An Elastic-visco-plastic Deformation Model and In Situ Micro-testing Of Al-Li: *Alexander Staroselsky*[1]; Luke Borkowski[1]; John Sharon[1]; [1]Utrc

Recent developments have produced a third generation of Al-Li alloys that provide not only weight savings, but also good fatigue performance, strength and toughness combination and compatibility with standard manufacturing techniques. Analyses of 3D microstructure and its correlation with properties need to be performed to determine optimal material processing. We develop physics based models for prediction of microstructure evolution and material properties of Al-Li alloy 2070. An elastic-plastic crystal plasticity model is developed and incorporated in finite element software. The model accounts for microstructural evolution during non-isothermal non-homogeneous deformation and is coupled with the damage kinetics. It bridges the gap between dislocation dynamics and continuum mechanics scales. Model parameters have been calibrated against lab tests including micro-pillar in-situ simple compression and simple shear tests. We present detail description of these nano-scale characterization in-situ testing. Numerical predictions are verified against the lab results including stress-strain curves and crystallographic texture evolution

5:00 PM

On the Dislocation Content of Random Grain Boundaries in Full 3D: *Diana Farkas*[1]; Bryan Kuhr[1]; [1]Virginia Tech

The dislocation content within the structure of random fully 3D grain boundaries in an FCC polycrystal was investigated through Molecular Dynamics modeling and the Dislocation Extraction Algorithm (DXA) for detecting lattice dislocations. It was found that a large fraction of the boundaries studied contained significant numbers of lattice dislocations as part of their structure, mostly Shockley partial dislocations and perfect lattice dislocations. The observed dislocation content varied widely depending on specific boundary geometrical parameters and relaxation state. Virtual tensile straining of these samples revealed how the dislocation content changed as a function of the strain applied to the sample. The results are discussed in the context of the role of the multiplicity of possible grain boundary structures on the deformation response of polycrystalline materials.

5:20 PM

3D Characterization of Dislocations in an Al-Cu-Mg Alloy: *Zongqiang Feng*[1]; Chengwei Lin[1]; Guilin Wu[1]; Xiaoxu Huang[1]; [1]Chongqing University

Quantitative characterization of morphological and crystallographic features of dislocations and dislocation structures in crystalline materials is of great importance to fully understand many dislocation-related phenomena and processes. The advent and development of dislocation tomography provides new capability for three dimensional characterization of morphological features of dislocations. However, the coupling of morphological features with the crystallographic characteristics of dislocations is still lacking. In this study, we combined electron dislocation tomography and correlative crystallography analysis to achieve high throughput characterization of geometrical and crystallographic parameters of dislocations in a water-quenched Al-Cu-Mg alloy. The obtained results led to new insight into the formation mechanisms of different dislocation features in the quenched alloy.

5:40 PM

Characterization of 3D Dislocation Structure in Single Grains and Parent-twin Pairs of Uniaxially Deformed Polycrystalline Mg AZ31 Alloy Specimens: *Gyula Zilahi*[1]; Gábor Ribárik[1]; Sean Agnew[2]; Wei Wu[3]; Ulrich Lienert[4]; Tamás Ungár[1]; [1]Eötvös University; [2]University of Virginia; [3]The University of Tennessee; [4]Deutsches Elektronen-Synchrotron

Magnesium alloys became popular lightweight structural materials during the last two decades. However, poor formability at room temperature is a key issue. Easy slip systems with the shortest, a type Burgers vectors cannot accommodate compression or tension along the c axis. $\{10\bar{1}2\}$ $10\bar{1}\bar{1}$ type twinning is an important mechanism of c axis tension, however it can accommodate limited amount of strain and it allows for unidirectional shear only. Earlier TEM studies also confirmed the activation of c+a type dislocations. High angular resolution 3D individual crystal diffraction measurements were carried out at the 1-ID beamline of APS synchrotron at Argonne National Laboratory. 788 grains of three plastically deformed samples were analyzed. Possible parent-twin relationships were identified based on the 3 dimensional misorientations. Dislocation structures of individual grains are characterized in terms of Burgers vectors and edge or screw character dislocations. The results are discussed in terms of earlier experimental and modeling studies.

6:00 PM

Site-specific Property Maps of Additively Manufactured SS316L Using a Mesoscale, Multi-physics Modeling Framework: *Nadia Kouraytem*[1]; Carl Herriott[1]; Xuxiao Li[1]; Wenda Tan[1]; Vahid Tari[2]; Anthony Rollett[2]; Ashley Spear[1]; [1]University of Utah; [2]Carnegie Mellon University

The microstructure of additively manufactured (AM) metals has been shown to be quite heterogeneous and exotic compared to conventionally manufactured metals. Consequently, the effective mechanical properties of AM-metal parts are expected to vary both within and among different builds. This talk presents a multi-physics modeling framework for simulating process, microstructure, and properties of AM-metal volumes. The framework predicts 3D-microstructural nucleation for a multi-pass, multi-layer Selective Laser Melting (SLM) process. The solidified microstructure is automatically sub-sampled to perform virtual mechanical testing using crystal-plasticity FFT modeling. The effective stress-strain response of each sub-sampled volume is then automatically analyzed to extract effective mechanical properties, which are used to generate property maps showing the spatial variability of mechanical properties throughout the simulated-build volume. As a demonstration, the framework is applied to SLM SS316L volumes processed with different laser parameters. The multi-physics framework and property maps could provide a path toward qualification of AM-metal parts.

New Experimental and Analysis Methods II

Tuesday PM
June 12, 2018

Room: Lille Scene
Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

3:50 PM Invited

Accurate 3D Reconstruction of Nanomaterials Using Automated Discrete Electron Tomography: *Xiaodong Zhuge*[1]; [1]Centrum Wiskunde & Informatica

Electron tomography is an important technique for the investigation of 3D morphology of nanomaterials. This method, however, suffers from missing wedge artifacts due to a restricted tilt range, which limits the objectiveness and repeatability of quantitative structural analysis. Discrete tomography is a promising reconstruction techniques for materials science, capable of delivering accurate reconstructions by exploiting the prior knowledge of material compositions. However, the application of discrete tomography remains challenging and it is often difficult to obtain consistent reconstructions from experimental datasets. In this work, we present the application of a new reconstruction technique, TVR-DART, for discrete electron tomography. It is demonstrated via experimental datasets that this technique is capable of consistently delivering reconstructions with significantly reduced artifacts and can automatically estimate its parameters. This new development promises to provide the electron microscopy community with an robust tool for high-fidelity 3D characterization of nanomaterials.

4:20 PM Invited

Correction of Artificial Density in 3D Reconstructed Micron-Sized Materials Induced by Nonlinear TEM Image Intensity: *Jun Yamasaki*[1]; Yuya Ubata[1]; Kazutoshi Murata[2]; Kazumi Takahashi[3]; Shin Inamoto[3]; Ryusuke Kuwahara[4]; [1]Osaka University; [2]National Institute for Physiological Science; [3]TORAY research center; [4]Okinawa Institute of Science and Technology Graduate University

Quantitative 3D reconstruction by tilt-series tomography needs a data set of projection images in which signals are proportional to integration of the sample structure to each direction. Ideally, image intensity in transmission electron microscopy (TEM) shows exponential attenuation with increasing thickness and thus taking the log gives linear signals. However, in practice, the attenuation deviates from such an exponential curve because of multiple scattering events of the incident electrons especially in micron-thick materials. Using a micron-sized carbon material, we explicitly showed that the deviation induced artificial density in the reconstructed volume. Moreover, we found that the actual attenuation curves were expressed by a function form with a few parameters. Based on total variation regularization for the reconstructed volume, we succeeded in iterative optimizations of the parameter values, which were used for the intensity corrections. As the result, internal structures of a yeast cell appeared more clearly than before the corrections.

4:50 PM
Characterization of Crystallographic Interface Character in Additively Manufactured 316L Stainless Steel: *David Rowenhorst*[1]; Lily Nguyen[1]; Richard Fonda[1]; [1]The US Naval Research Laboratory

Additive Manufacturing (AM) shows great potential for the rapid manufacturing of low volume parts at lower costs. Understanding the microstructural evolution of these materials is of interest since a post-build heat treatment is often used to develop desired properties, thus understanding and predicting the development of these microstructures is essential for understanding the resultant properties of a build. In this presentation, we will show how serial EBSD sections of as-built AM 316, were collected with an automated serial sectioning system, and then present how the distorted EBSD maps were aligned, stacked and reconstructed to make a consistent 3D dataset. We will also discuss data analysis methods for the highly misoriented grains within the structure, and provided the full five parameter grain boundary character distributions for the AM material, and compare the results to those found in our results of traditionally processed 316L.

5:10 PM
Estimating the Fibre Length Distribution Using the Fibre Endpoint Process: *Jan Niedermeyer*[1]; Claudia Redebach[1]; [1]TU Kaiserslautern

The mechanical strength in fibre reinforced polymers is governed by the length and orientation distribution of the fibres. Estimating the fibre length distribution in fibre reinforced polymers from CT data is still a challenge. Image quality usually does not allow a full fibre segmentation. Using Gaussian curvature we can segment the fibre endpoints from a CT image. By interpreting these endpoints as a point process we can then use point process statistics to investigate properties of the underlying fibreprocess. We will investigate methods using point process statistics to estimate the fibre length distribution.

5:30 PM
Software Developments for Reduction of High Energy Diffraction Microscopy Data: Hemant Sharma[1]; Peter Kenesei; Jun-Sang Park; *Jonathan Almer*; [1]Argonne National Laboratory

High Energy Diffraction Microscopy (HEDM) technique is used for non-destructive in-situ characterization of polycrystalline materials during thermo-mechanical treatments. This talk will outline the developments to the MIDAS software for reduction of both Near Field and Far Field HEDM data. We have recently implemented a real-time streaming pipeline for remote data reduction at Sector 1, APS. We will present a comparison of two different approaches for grain tracking during sample evolution: one using diffraction peaks and the other using grain orientations. The applicability of each approach in different cases will be discussed. In addition, a robust methodology for detection of twins in FCC materials will be presented.

5:50 PM
Graph Techniques for Image Segmentation: *Olumide Okubadejo*[1]; [1]Universite Grenoble, Alpes

Segmentation techniques have overtime evolved in their ability to detect grains in tomography images depicting mechanical processes. Algorithms such as watershed have proven to be extensively useful for the detection and characterisation of these grains. However, it is limited in the fact that it provides a solution based on an analogical representation of the problem. This makes scaling our current solutions in 3D formulations to 4D formulations potentially difficult. I present the use of alternative approaches, specifically Graph based techniques which have symbolic representations and hence give a wider degree of freedom in our holistic understanding of the problem and thus, our solution to it. I also propose graph energy minimisation techniques as solutions to 4D segmentation problems

Measuring and Predicting Grain Shapes, Sizes, Crystallography, and Spatial Distributions I

Wednesday AM
June 13, 2018

Room: Lille Scene
Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

8:00 AM Invited
Multiscale Multimodal Correlative 3D Imaging of Biomaterials: David McComb[1]; *Isabel Boona*[1]; Shaz Khan[2]; Jonathan Earl[2]; [1]The Ohio State University; [2]GlaxoSmithKline Consumer Healthcare R&D

Many materials challenges require an understanding on multiple length scales and often visualization in three dimensions (3D) is essential. For example, composites found in lithium ion batteries, catalytic systems and even mineralized tissue are comprised of organic and inorganic phases with many channels, pores, and features that span length scales from centimeters to nanometers. Fully characterizing these complex structures requires the use of correlative microscopy applied to a sufficiently broad range of techniques that can span the full range of length scales involved. In this contribution we will discuss development of a multiscale multimodal correlative workflow that combines X-ray microtomography (XMT) with FIB-SEM and scanning transmission electron microscopy (STEM). The workflow process developed allows us to take correlate information from the atomic scale to the macroscopic scale on the same specimen. Our goal is to understand the 3-D structure of human dentin and the relationship between the structure and properties.

8:30 AM
Twin Related Domain Structure in a Polycrystalline Nickel-base Superalloy: *William Lenthe*[1]; Jean-Charles Stinville[2]; McLean Echlin[2]; Toby Francis[1]; Tresa Pollock[2]; [1]Carnegie Mellon University; [2]University of California, Santa Barbara

Fatigue is the life limiting property for the polycrystalline nickel based superalloys. René 88DT exhibits a high density of annealing twin boundaries and favorably oriented twin boundaries in large grains serve as fatigue crack initiation sites. Although the importance of twin boundaries has been established, their 3D structure and connectivity is poorly understood. Multiple 3D volumes of René 88DT have been collected via femtosecond laser serial section using the TriBeam system. New metrics to quantify twin related domain structure have been developed and applied to hundreds of fully captured domains with implication for fatigue lifetime examined.

8:50 AM
A Full 3D Description of the Structural Formation of the Prismatic Tissue in Marine Shells Using Classical Laws from Materials Science: *Dana Zöllner*[1]; Igor Zlotnikov[1]; [1]TU Dresden

Polycrystalline networks forming the microstructures of many materials have an immense impact on materials behavior. Hence, many attempts have been made to understand and consequentially predict microstructures and their changes during grain growth analytically. A special case that has been drawing much attention is ideal grain growth, where all grain boundaries are characterized by the same properties, for which over the years many analytic laws have been derived in two and three dimensions.In the present work, we show that the formation of the prismatic layer in marine shells like Atrina vexillum can be described fully by classical analytical approaches from various physical theories. In particular, we quantitatively analyze the three-dimensional structure of the prismatic assembly in Atrina vexillum and show that while the average grain size follows a square-root law, the polycrystalline microstructure is in a self-similar state fulfilling consistently among others the well-known von Neumann-Mullins law.

9:10 AM
4D Imaging of Silicon-Molybdenum Alloyed Ductile Cast Iron Including Results from DVC Analysis: *Torsten Sjögren*[1]; Stephen Hall[2]; Erik Dartfeldt[1]; Peter Skoglund[3]; Lennart Elmquist[4]; Jessica Elfsberg[3]; Marta Majkut[5]; [1]RISE Research Institutes of Sweden; [2]Lund University; [3]Scania CV AB; [4]Swerea SWECAST; [5]European Synchrotron Radiation Facility

Ductile Cast Iron (DCI) materials are used in the heavy truck industry where increasing environmental requirements inevitably lead to increased combustion pressure and temperature that, in turn, entail more severe loading of the structural materials. In-situ tensile loading of DCI samples has been carried out at ID11 of ESRF with 4D x-ray tomography and 3D-XRD. The tomographic images have been analyzed using Digital Volume Correlation to assess the coupling between microstructural features of the material and its mechanical behavior. In addition, the data obtained from the 3D-XRD is used to study how the grain structure including the properties of individual grains influences the deformation and failure. The knowledge gained in the study will be used to improve the utilization of the DCI material in truck components, including by using the new insight to develop computational models that take the material microstructure into account.

9:30 AM
Revealing 3D Microstructures with High-energy X-rays: *Jonathan Almer*[1]; Peter Kenesei[1]; Jun-Sang Park[1]; Hemant Sharma[1]; Meimei Li[1]; Paul Shade[2]; Stuart Stock[3]; [1]Argonne National Laboratory; [2]Air Force Research Laboratory; [3]Northwestern University

High-energy x-rays from 3rd generation synchrotron sources, including the Advanced Photon Source (APS), possess a unique combination of high penetration power and spatial, reciprocal space, and temporal resolution. These characteristics, coupled with extensive worldwide efforts over the past decades, have produced a variety of 3D imaging techniques using both density and diffraction/scattering contrast. Within the X-ray Science Division at the APS, we have focused on combining several of these techniques to study polycrystalline materials through (i) absorption-based tomography, (ii) high-energy diffraction microscopy (HEDM or 3DXRD) and (iii) scattering tomography. The latter two approaches are complementary, as HEDM provides diffraction information (strain, orientation, shape and size) of individual grains in aggregates while scattering tomography yields spatially resolved but grain-averaged information, particularly relevant for fine-grained materials below HEDM limits. Use of these techniques for in situ studies of biological systems, aerospace and nuclear-relevant materials will be presented, along with descriptions of some enabling in situ equipment. Further development of these techniques will be discussed, both prior to and after the planned APS upgrade to a diffraction-limited source.

9:50 AM Break

Phase Transformations, Particle Coarsening, Grain Growth, and Recrystallization III

Wednesday AM
June 13, 2018

Room: Store Scene
Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

8:00 AM Invited
3D Continuum Theory of Defects and Microstructure under Irradiation: *Anter El-Azab*[1]; [1]Purdue University

Irradiation drives materials away from equilibrium by creating point defects at densities much higher than their equilibrium concentrations. Defects diffuse and interact in the material, which leads to microstructure changes and dimensional changes. Although these phenomena originate by one and the same process, which is defect generation, they are often modeled separately. We present a unified theoretical framework for defect and microstructure dynamics under irradiation based upon non-equilibrium thermodynamics. This approach is based on the balance principles of mass, momentum and energy, and the use of the second law of thermodynamics. These principles result in the kinetic equations of point defects at the scale of microstructure, the mesoscale heat equation and stress equilibrium equation. The concepts of continuum mechanics are invoked to describe dimensional changes in the irradiated material. The main features of this framework will be presented along with specific examples related to the irradiation response of single crystals.

8:30 AM
Integrated Imaging in Three Dimensions: The Sum is Greater than the Parts: Ron Keinan[1]; Hrishikesh Bale[2]; Nicolas Gueninchault[3]; Erik Lauridsen[3]; *Ashwin Shahani*[1]; [1]University of Michigan; [2]Carl Zeiss X-ray Microscopy, Inc.; [3]Xnovo Technology ApS

Recent developments in laboratory-based diffraction contrast tomography (LabDCT) have shown its capability to non-destructively map the 3D morphology and crystallographic orientation in the bulk of a polycrystalline sample. Using a combination of LabDCT and attenuation-based tomography, we present here the first experimental results from the imaging of a polycrystalline silicon sample and demonstrate the application of this integrated approach in obtaining crucial microstructural and grain related crystallographic information. It is anticipated that our integrated approach can be extended to other microstructures that are simultaneously multiphase and polycrystalline.

8:50 AM
3D Laboratory Diffraction Contrast Tomography Study of Nucleation in Al-1%Si: *Jun Sun*[1]; Yubin Zhang[2]; Nicolas Gueninchault[1]; Florian Bachmann[1]; Allan Lyckegaard[1]; Erik Lauridsen[1]; Dorte Juul Jensen[2]; [1]Xnovo Technology; [2]Technical University of Denmark

3D methods have opened new avenues for recrystallization studies and revealed that much accepted 'knowledge' does not match what is seen in 3D. This work deals with nucleation within multi-phase metals. Numerous electron microscopy studies have investigated effects of parameters such as size and distribution of second-phase particles on particle stimulated nucleation (PSN) and PSN is 'known' to be the major nucleation mechanism in many materials. The novel laboratory diffraction contrast tomography (LabDCT) technique allows non-destructive 3D orientation mapping of crystalline materials. In this study, we applied LabDCT to characterize the nuclei in lightly annealed 50% cr Al-1%(wt) Si. The 3D distribution of particles and nuclei are mapped, revealing that the particles are not the major nucleation site. Only Si particles clustered along the prior grain boundaries are observed to be preferential nucleation sites. This result is discussed and orientation relationships between the nuclei and the neighboring deformed matrix are analyzed.

9:10 AM
Measuring Anisotropic Grain Boundary Mobilities by Bridging 3D Experiments and Simulations: *Jin Zhang*[1]; Peter Voorhees[2]; Henning Poulsen[1]; [1]Technical University of Denmark; [2]Northwestern University

We propose a fitting approach to measure the anisotropic reduced grain boundary mobilities by comparison between time-resolved 3D x-ray experiments and 3D phase-field simulations. The grain growth in pure iron is measured by diffraction contrast tomography (DCT). With one timestep from the experiment as input, the phase-field method is used to simulate the evolution of grain growth. The dissimilarity between experiment and simulation is characterized by a cost function. The values of the reduced mobilities that minimize the cost function are regarded as the physical values of the materials parameters. The fitting approach is formulated as an optimization problem and is solved iteratively. In each optimization iteration, the original optimization problem is approximated by a series of sub-problems, which are solved individually. The fitting approach is demonstrated on synthetic datasets and then applied to the DCT dataset to measure the reduced mobilities as a function of the grain boundary misorientation.

9:30 AM
Atomistic Simulation and Phase Field Modeling Studies on the Three-Dimensional Growth Pattern Formation of Magnesium Alloy Dendrite: *Jinglian Du*[1]; Ang Zhang[1]; Zhipeng Guo[1]; Manhong Yang[1]; Shoumei Xiong[1]; [1]Tsinghua University

The 3D pattern formation of magnesium alloy dendrite was investigated using phase field simulations in light of an anisotropic function model developed based on the experimental findings and spherical harmonics. The anisotropic parameters involved in the anisotropy function model were quantified via relevant atomistic simulations based on density functional theory and hexagonal lattice structure. It was found that the simulated results of dendritic growth pattern were in good correspondence with the experimental findings on the 3D dendritic morphology with 18-primary-branch of most magnesium alloys, including Mg-Al, Mg-Ba, Mg-Ca, Mg-Y and Mg-Sn. Furthermore, the 3D morphological transition of Mg-Zn alloy dendrite from 18-primary-brach to 12-primary branch observed in experiments is closely related to the growth parameters, such as supercooling, anisotropic strength and partition coefficient. Our investigations provides a pathway to enhance one's understanding on 3D growth pattern of magnesium alloy dendrite from phenomenological descriptive picture to a more intrinsic predictive way.

9:50 AM Break

Measuring and Predicting Grain Shapes, Sizes, Crystallography, and Spatial Distributions II

Wednesday AM
June 13, 2018

Room: Lille Scene
Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

10:20 AM Invited
Dark-field X-ray Microscopy in the Shadow of Biominerals: *Phil Cook*[1]; Jean-Pierre Cuif[2]; Yannicke Dauphin[2]; Carsten Detlefs[1]; Elise Dufour[3]; Anders Jakobsen[4]; Mustafacan Kutsal[1]; Henning Poulsen[4]; Vanessa Schoeppler[5]; Hugh Simons[4]; Can Yildirim[1]; Igor Zlotnikov[5]; [1]ESRF; [2]Muséum nationale d'Histoire naturelle; [3]UMR 7209 CNRS/MNHN; [4]Danish Technical University; [5]BCUBE

We have examined biominerals using dark-field x-ray microscopy and will illustrate new perspectives on their microscale crystalline properties. Dark-field x-ray microscopy allows multiscale in situ diffraction topography imaging of biomineral fibres (~100 µm), bundles (~10 µm), and their component prismatic crystalline units (~1 µm) using Bragg diffracted beams with a 100 nm real space resolution, 0.001° angular resolution, and strain resolution of 10^-5.We describe several examples studied at the recently commissioned instrument at ESRF ID06. In fish otoliths, we present bulk analyses of crystalline bundles, revealing the relative orientation relations of the prismatic crystals as well as internal variations in orientation and strain. In a Pinctada shell prism we show that, while it is quasi-monocrystalline, there are variations in crystallite orientation on the order of 10^-3 degrees along with strain variations on the order of 10^-5. We investigate the relation of habits of biomineral crystals and internal strains.

10:50 AM
3D TEM Characterization of Polycrystalline Metals: *Xiaoxu Huang*[1]; Qiongyao He[2]; Zongqiang Feng[2]; Guilin Wu[2]; Søren Schmidt[1]; [1]Technical University of Denmark; [2]Chongqing University

Mechanical properties of polycrystalline metals are determined by their microstructural, crystallographic and chemical parameters. Recent development of electron tomography, 3D orientation mapping and 3D atom probe has enabled precise characterizations of a diversity of 3D microstructural, crystallographic and chemical information from a variety of materials, which offers new opportunities for 3D materials science of polycrystalline metals at nanoscale. In this presentation, the progresses in developing TEM-based 3D orientation mapping and dislocation tomography techniques are demonstrated by showing examples obtained in polycrystalline metals. New challenges will be disccused with respect to the development of sample stage and reconstruction software for a full and precise 3D characterization of microstructural and crystallographic parameters.

11:10 AM
Finite Element Simulation of Grain Growth with an Arbitrary Grain Boundary Energy: *Erdem Eren*[1]; Jeremy Mason[1]; [1]University of California, Davis

Three-dimensional microstructure reconstructions and grain boundary energy reconstructions provide input and validation data that could dramatically improve simulations of microstructure evolution. Unfortunately, there are few simulations that can make full use of this data in the literature. We have developed a finite element simulation that (1) uses a volumetric mesh to allow the eventual inclusion of arbitrary material physics, (2) significantly expands the set of allowed topological transitions to allow for general grain boundary network dynamics, and (3) proposes an energy dissipation criterion to select a topological transition in a system with arbitrary grain boundary energy. This talk will mainly focus on the second and third points, since they seem to be novel in the literature. The resulting finite element code (based on SCOREC by the Rensselaer Polytechnic Institute) is expected to improve the ability of simulations to reproduce recently available experimental observations of microstructure evolution in three dimensions.

11:30 AM
Missing Information and Data Fidelity in Digital Microstructure Acquisition: *Mo Li*[1]; [1]Georgia Institute of Technology

Microstructure is one of the pillars supporting the structure-property relations in materials science and engineering. Its digitized format, the digital microstructure, plays an increasingly vital role in materials genome, new architecture design and advanced manufacturing of functional materials. Despite the efforts in the past decade, one basic issue facing digital acquisition of microstructures is left untouched, that is, how much information is missing in the first step of data gathering and processing. Here using a polycrystal model and new microstructure characterization methods, we show quantitatively the missing information and related data fidelity. The lost microstructural data could become significant depending on the experimental resolution and the nature of the microstructures. We also discuss the uncertainties and deviations in the predicted material properties caused by the lost microstructural information.

New Experimental and Analysis Methods III

Wednesday AM
June 13, 2018

Room: Store Scene
Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

10:20 AM Invited
Tomographic Atomic Force Microscopy: *Bryan Huey*[1]; [1]University of Conneticut

10:50 AM
Identifying and Quantifying Anomalies and Rare Events in Large Volume 3D Polycrystalline Aggregates: *Sean Donegan*[1]; Michael Uchic[1]; Michael Groeber[1]; Michael Chapman[2]; Adam Pilchak[1]; [1]Air Force Research Laboratory; [2]UES, Inc.

Understanding the behavior of anomalies and rare events in polycrystalline aggregates is important for predicting macroscale behavior in many materials systems. Statistical analysis of such outlier features usually lacks predictive merit due to small characterization volumes coupled with the rarity of the interesting events. Recent advances using polarized light microscopy and serial sectioning allow for the characterization of large-volume 3D data sets in optically anisotropic materials. This data collection pipeline, described in detail in a complementary submission to the congress, enables the characterization of more than 100,000 unbiased grains in a single phase alpha titanium alloy, offering unique opportunities for exploring outlier features in a polycrystalline structure. We present several statistical techniques from extreme value theory for quantifying outliers in microstructure feature distributions, such as grain size and morphology. Additionally, we highlight the advantages of a monolithic 3D data set, including the use of sub-sampling for cross-validation of statistical models.

11:10 AM
Efficient Pathways for 3D Characterization of Rarely-occurring Features in Polycrystalline Ensembles: *Michael Uchic*[1]; Michael Chapman[2]; Sean Donegan[1]; Michael Groeber[1]; Adam Pilchak[1]; [1]Air Force Research Laboratory; [2]UES, Inc

Characterization of rarely-occurring features in 3D polycrystalline ensembles is a generally unexplored topic, in large part because of the current difficulty in collecting experimental datasets that allow for meaningful statistical analysis. The recent development of computationally-controlled polarized light imaging—which was presented at 3DMS 2016—has enabled more efficient data collection protocols to gather both grain morphology and some aspects of crystallographic orientation in optically-anisotropic metals such as titanium. This study presents the combined use of this technology with mechanical polishing-based serial sectioning instrumentation to produce 3D data sets from single phase alpha titanium samples that contain more than 100,000 unbiased grains. We present key aspects of the data collection and post-processing pipeline that enable a fully-automated workflow, and, highlight results of the analysis of the tails of the grain size distribution using extreme value theory, which is described in detail in a complementary submission for this congress.

11:30 AM
A New End Station at the Materials Science Beamline at the ESRF: *Jonathan Wright*[1]; Marta Majkut[1]; Pavel Sedmak[1]; Carlotta Giacobbe[1]; Wolfgang Ludwig[1]; Thomas Buslaps[1]; Henri Gleyzolle[1]; Ludovic Ducotte[1]; [1]ESRF

A new end-station for high-energy X-ray nanofocus measurements has been installed at the ID11 beamline at the ESRF. The instrument offers beam sizes in the range 100nm – 1 micron and has a diffractometer that can align and maintain samples in the X-ray beam during rotation. The instrument offers a full suite of single crystal, powder, PDF and grain mapping measurement options. XRD-CT data collection is accessible with relatively high frames rates (>25 fps) and 2D slices can be stacked to get a 3D view of the sample. The instrument has completed user experiments in various scientific areas already, including metallurgy, ceramics, chemistry and geology. Existing software has been adapted to allow reconstruction of the spotty XRD-CT data. We will discuss some of the scientific highlights from this new end-station and future perspectives in the light of the forthcoming ESRF source upgrade.

11:50 AM
X-ray Diffraction Contrast Tomography and Applications to 3D Materials Science: *Wolfgang Ludwig*[1]; Nicola Vigano[2]; [1]Université de Lyon; [2]Centrun Wiskunde Informatica

X-ray diffraction contrast tomography is a fast orientation mapping technique applicable to a variety of polycrystalline materials. Spatially resolved orientation maps are reconstructed on a grain by grain basis using an iterative 6D optimization scheme. Recent extensions of the model include a number of physical corrections (detector point spread, beam profile, attenuation) and improved handling of simultaneous reconstruction of orientation related domains. We will showcase the current possibilities and limitations on a series of selected application examples covering in-situ studies of recrystallization, grain growth, plastic deformation and phase transformations.

Measuring and Predicting Grain Shapes, Sizes, Crystallography, and Spatial Distributions III

Wednesday PM
June 13, 2018

Room: Store Scene
Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

1:30 PM Invited
3D Modeling and Simulations of Morphologies in Filler-filled Rubbers: *Katsumi Hagita*[1]; [1]National Defense Academy

Filler-filled rubber is of great interest as a system in which the 3D structure of fillers in a volume from nanometer to micrometer dimensions greatly influences the structure-property relationships. For tire rubbers, primary shape of the filler can be regarded as a sphere whose diameter is a few ten nanometer. Morphologies of the spheres in a volume of micro-meter dimension have important roles on properties. Recently, we have adopted a broad approach to grasping the morphology in large volume. A real space approach is Focused Ion Beam Scanning Electron Microscopy (FIB-SEM) observations. A reciprocal space approach is Reverse Monte Carlo modeling of 3D positions of the spheres from ultra-small-angle X-ray scattering profiles observed in the synchrotron radiation facility SPring-8. Very recently, we confirmed consistency of the two approaches by evaluating scattering profile from the FIB-SEM data. We also performed large-scale coarse-grained molecular dynamics simulation to study the structure-property relationships.

2:00 PM
The Digital Twin – A Comparative Study of Material Simulation on µCT-Scanned and Modelled Microstructures: *Constantin Bauer*[1]; Aaron Widera[1]; Tim Schmidt[2]; Florian Schimmer[2]; [1]Math2Market GmbH; [2]Institut für Verbundwerkstoffe GmbH

Digital material engineering has recently become essential for many industrial applications. The simulation tools ability to create realistic representative microstructure models and to determine their physical material properties, helps in profitably quicken product development. The simulation software GeoDict is a straightforward solution for digital material analysis, engineering, and optimization.The materials' microstructure is obtained either through import and segmentation of µCT-scans or by modelling the microstructure from direct input of material parameters. Both modelling approaches are provided by GeoDict and compared in this work. A continuous glass fiber reinforced fabric with thermoset matrix is scanned. The µCT-scans are imported into GeoDict and segmented to create a microstructure model. Mechanical and flow simulations, carried out on the microstructure model, determine its stiffness and permeability. As alternative, a digital twin of the material is modelled from input parameters and the simulation results are compared to those of the µCT-scan model.

2:20 PM
Simulation of Material Properties Directly on CT Scans: *Karl-Michael Nigge*[1]; Johannes Fieres[1]; Philipp Schumann[2]; [1]Volume Graphics GmbH; [2]Concept Laser GmbH

Classical FEM simulations may not always be well suited for micromechanical simulations of complex materials because they require the generation of geometry conforming meshes which must be fine enough to capture all relevant geometric details and coarse enough to keep the computational effort at a practical level on the other hand. Recently, mesh-less and immersed-boundary finite element methods have been used to overcome this meshing problem. In order to validate this simulation approach, a comparison between experimental and simulated results of tensile tests was conducted for material probes with complex internal structures, showing a good agreement. The approach was also validated successfully against a classical FEM simulation for a solid cube and a cubic lattice made. The simulation approach can be used to determine the effective mechanical properties of new materials with inherently complex internal structures.

2:40 PM
Aggregate Presence and Impact of 3-dimensional Defect Populations in Additively Manufactured Stainless Steel: *Jonathan Madison*[1]; Laura Swiler[1]; Stephanie DeJong[1]; Thomas Ivanoff[1]; Brad Boyce[1]; Bradley Jared[1]; Jeffrey Rodelas[1]; Bradley Salzbrenner[1]; [1]Sandia National Laboratories

The salient relations between performance and processing defects of additively manufactured metals can be difficult to discern and often somewhat elusive to verify. To address this challenge micro-computed tomography was applied to an ensemble set of 100+ additively manufactured tensile samples of stainless steel. Tomographic datasets having resolutions of 10.2 microns per cubic voxel edge, or better, are utilized to identify and measure process-induced internal defect structure prior to mechanical testing. In this study, porosity and lack of fusion defects are the primary features of interest. Individual sample and aggregate build distributions for defect size, shape and spatial arrangements are reported in terms of their statistical presence. Correlations in observed defect presence will be shown and their relation to high-throughput mechanical testing results will also be highlighted.

3:00 PM Break

Phase Transformations, Particle Coarsening, Grain Growth, and Recrystallization IV

Wednesday PM
June 13, 2018

Room: Lille Scene
Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

1:30 PM
Quantification of Inter Diffusion for Ceramic/Metal Interface with 3D-SIMS: *Lei Zhang*[1]; Chunli Dai[1]; Jie Zhang[1]; [1]Institute of Metal Research, Chinese Academy of Sciences

Layering images of diffusion species by TOF-SIMS analysis can be reconstructed in 3D and reveal chemical information at interfaces with resolution down to nanometer in both lateral and longitudinal direction. This 3D-SIMS analytics tool facilitates the quantification of Inter diffusion of ceramic/metal interfaces, which is crucial to tell the bonding in between. In terms of the 3D-SIMS views of Al+, Cr+ and Zr+ ions in the TiAlC coating and Zr substrate, diffused Al and Cr were clearly observed in both as-deposited and annealed states. Quantification results of stoichiometric ratio indicated that Cr diffused more than Al. By Gaussian convolution of the 3D-SIMS data, the counts density of investigated species was transformed into quasi-concentration space. The concentration contour can be given and exhibited the relationship relative to the initial interface in 3D view. It shows that the diffusion front was uneven and Cr diffused more and further than Al.

1:50 PM
Three Dimensional Synchrotron Characterization of Neutron Irradiated Metallic Fuels: *Maria Okuniewski*[1]; Jonova Thomas[1]; Sri Nori[1]; Alejandro Figueroa[1]; Peter Kenesei[1]; Jun-Sang Park[1]; Hemant Sharma[1]; Jon Almer[1]; [1]Purdue University

Metallic fuels are utilized in both nuclear research and test reactors, as well as fast reactors. Typical metallic fuel alloys include uranium alloyed with either molybdenum or zirconium, which stabilizes the body-centered cubic phase during irradiation. The fuel geometries and operational conditions vary widely for these materials. High energy x-rays have been utilized to assess the microstructural changes of the UMo and UZr fuels that have undergone neutron irradiation at various fluences and temperatures. Synchrotron tomography was utilized to determine porosity, phase regions, and diffusion barrier stability. High energy diffraction microscopy provided insight into the grain morphologies, center of mass, and orientation. These results will be compared to electron microscopy.

2:10 PM
3D-XRD Study of Phase Transformation Microstructures in Deep Earth Minerals: *Sebastien Merkel*[1]; Christopher Langrand[1]; Angelika Rosa[2]; Volodymyr Svitlyk[2]; David Dobson[3]; Nadège Hilairet[1]; [1]Universite de Lille; [2]ESRF; [3]University College London

Hydrostatic pressure has a profound effect on the properties of materials. In the Earth's mantle for instance, minerals undergo series of phase transformations with implications for its structure and dynamics. Here, we use multigrain crystallography combined with high pressure / high temperature experiments in diamond anvil cells in order to asses the effect of phase transformations on deep Earth minerals microstructures. We focus our study on a perovskite (Pv) to post-perovskite (pPv) transformation, both orthorhombic structures. A polycrystal of NaCoF3 is compressed up to 30 GPa at 900 K, inducing the Pv-pPv transformation, and decompressed, inducing the reverse transformation. Using in-situ measurements, we study the induced microstructures (grain orientations, grain sizes, etc) and the corresponding transformation mechanisms. The results have important geophysical implications. They also demonstrate the relevance of the technique for other geophysical systems but also in other scientific fields for which high pressure transformation microstructures are relevant.

2:30 PM
Internal Stress and Damage Evolution during Loading of Additively Manufactured Stainless Steel: *Bjørn Clausen*[1]; Reeju Pokharel[1]; Timothy Ickes[1]; Darren Pagan[2]; Joel Bernier[3]; Donald Brown[1]; George Gray[1]; [1]Los Alamos National Laboratory; [2]Cornell University; [3]Lawrence Livermore National Laboraotry

Additive manufacturing (AM) of metals has the potential to revolutionize the manufacturing industry; however, significant challenges remain before it can be qualified as a transformative metal component fabrication technique. We will present the results of in-situ HEDM and tomography measurements during tensile loading of as-built and heat treated AM 304L stainless steel (SS). The measurements were performed using the RAMS2 load frame on the F2 instrument at CHESS. Near-Field, Far-Field HEDM and tomography were invoked for the heat treated AM SS to monitor the development of internal stresses and void/fracture. The initial microstructure of the as-built AM SS did not lend itself to HEDM measurements as the grain size is very small and the dislocation density is relatively high, but powder diffraction measurements of average internal stress and texture as well as tomography measurements to determine the void formation and fracture of the material was applied during the loading.

2:50 PM
Coarsening Statistics in an Iron Polycrystal and Advances in Grain Boundary Energy Extraction: *Yu-Feng Shen*[1]; Xiaoting Zhong[1]; He Liu[1]; Aditi Bhattacharya[1]; Gregory Rohrer[1]; Robert Suter[1]; [1]Carnegie Mellon University

Near-field High Energy x-ray Diffraction Microscopy (nf-HEDM) is used to track the three dimensional microstructural evolution of an alpha phase iron sample under thermal annealing. We study the evolution of grain and grain boundary statistics. By matching grains across the two measured states, we track thousands of grains as they evolve, along with the movements of grain boundaries. Further, we present new solution methods and a new algorithm for extracting relative grain boundary energies based on observations of large numbers of triple junction topologies. Accelerated convergence of the original Morawiec formulation of the problem is achieved with modern optimization methods. A new formulation will be presented that avoids the limitations of binning of the five dimensional space of grain boundary character.

3:10 PM Break

Wednesday Plenary

Wednesday PM
June 13, 2018

Room: Store Scene
Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

3:20 PM Plenary
Challenges in Acquisition of Statistically Significant Multimodal 3D Data for Property Prediction: William Lenthe; Andrew Polonsky; McLean Echlin; Jean-Charles Stinville; *Tresa Pollock*[1]; [1]University of California, Santa Barabara

The development of high fidelity material property and life prediction models often requires three-dimensional information on the distribution of phases, interfaces, grains or extrinsic defects. Acquisition of this information requires consideration of appropriate representative volume elements that vary in size with material, microstructure and the property of interest. Recent advances in the use of femtosecond lasers for layer-by-layer ablation within the TriBeam microscope platform to gather representative volumes of information will be reviewed. Examples of the utility of multimodal data will be given for several classes of materials. Statistical measures of convergence for microstructural features and their relationship to convergence volumes for properties will be considered. The challenges for integrating experimental voxelized data with models for prediction of mechanical properties will be addressed for nickel-base and titanium-base alloys.

4:05 PM Question and Answer Period

4:20 PM Break

Posters

Monday PM
June 11, 2018

Room: Store Scene
Location: Kulturværftet (Culture Yard) Conference Center

Session Chair: To Be Announced

P-1: Porosity Analysis of AM Powder based on Machine Learning Approach: *He Liu*[1]; Yufeng Shen[1]; Robert Suter[1]; [1]Carnegie Mellon University

The properties of porosity within AM powder will affect the quality of final product. A 3-D segmentation and analysis method based on machine learning approach was developed to analyze the porosity and size distribution of AM powders. Powders and pores are segmented and recognized in three dimensional volume data to increase accuracy. Valuable statistical information can be extracted to evaluate the quality of AM powder. This will give a quantitative guide for the selection of AM powder for manufacturing. Same technique could be applied to other 3D dataset to extend the application.

P-2: 3D Multigrain Crystallography for Detection and Discrimination of Secondary Phases in Cu2ZnSnS4 for Thin Film Solar Cell Applications: *Mariana Mar Lucas*[1]; Henning Poulsen[1]; Jens Andreasen[1]; [1]Technical University of Denmark

Cu2ZnSnS4 (CZTS) is a polycrystalline material for thin film solar cell applications. A CZTS layer typically presents secondary phases that form due to a thermodynamic equilibrium and the stoichiometry condition (Cu-poor, Zn-rich). They are difficult to identify, and thus, to quantify because of the similarity of their lattice parameters. This represents a major challenge to the common characterization techniques, i.e. XRD, Raman.[1] Multigrain crystallography provides structural characterization of polycrystalline materials. Utilizing 3D X-ray diffraction (3DXRD) microscopy, 3D maps of the grains can be generated visualizing their morphology, orientations, and strains. [2] By applying 3DXRD and using the latest indexing algorithms, it is intended to identify and quantify the secondary phases in CZTS films. References: [1] Berg, D. M. et al., Thin Solid Films 569, 113–123 (2014).[2] Poulsen, H. F., . J. Appl. Crystallogr. 45, 1084–1097 (2012).

P-3: 3D Recrystallization Studies of Aluminium Studied by Dark Field X-ray Microscopy: *Mustafacan Kutsal*[1]; Phil Cook[1]; Can Yildirim[1]; Carsten Detlefs[1]; Henning Poulsen[2]; [1]European Synchrotron Radiation Facility; [2]Technical University of Denmark

Three-dimensional studies of recrystallization in metals have generally been carried out by serial sectioning. Two-dimensional techniques such as optical or electron microscopy provide images or diffraction maps. These are then assembled in post processing to form 3D reconstructions. Clearly, such approaches cannot be used in situ and may suffer from surface modifications due to sectioning. Here, we present the use of Dark Field X-ray microscopy to track recrystallization in aluminium in situ. The technique employs Bragg diffraction of hard X-rays from individual deformed or recrystallized grains inside the 3D volume and provides real-space information by using an x-ray objective lens. This enables us to track transformations on a single grain inside the 3D volume with high angular and spatial resolution. Initial results on 3D mapping of subgrains, structure evolution during dissolution of deformed grains, and strain and misorientation relations in recrystallized grains will be presented.

P-4: 3D Visualization of Pores in Ti-6Al-4V Samples Manufactured by Selective Laser Melting Method with Heterogeneous Nucleation Site Particles: *Yoshimi Watanabe*[1]; Masafumi Sato[1]; Tadachika Chiba[1]; Hisashi Sato[1]; Naoko Sato[2]; Shizuka Nakano[2]; [1]Nagoya Institute of Technology; [2]National Institute of Advanced Industrial Science and Technology (AIST)

It is reported that the presence of defects dominates high cycle fatigue life in additively manufactured samples, where most fatigue cracks nucleate exclusively at pores rather than at other microstructural features. In our previous studies, effect of TiC heterogeneous nucleation site particles on microstructure of Ti-6Al-4V samples manufactured by selective laser melting (SLM) method was studied. It was found that the density of Ti-6Al-4V samples could be increased by addition of TiC particles, since uniform microstructure and suppression of pore formation could be achieved by heterogeneous solidification with heterogeneous nucleation site particles. In this study, the size, volume fraction and spatial distribution of the pores in Ti-6Al-4V samples, manufactured by SLM method with TiC heterogeneous nucleation site particles, have been characterized in 3D using x-ray computed tomography (XCT).

P-5: Application of Finite-element Crystal Plasticity for the Modeling of Microstructure Fragments of Titanium Alloys and Its Deformation Processes: *Andrey Musienko*[1]; [1]NRC «Kurchatov Institute» - CRISM «Prometey»

Recently virtual schema based on observations of material microstructure realized using computer. Internet made them available. Author was interested in finite element plasticity of crystals, virtual aggregate of 27 Voronoï polyhedrons was seen for example. Creation of the virtual models is replaced by questions of usefulness of their application in materials science. For (a+ß) titanium alloys different microstructures are observed. Interested in mechanical stresses and deformations, possible to carry out computation with finite-element method, digitizing images of a microstructure. One can consider crystallographic orientations corresponding to really measured.Formation of virtual structures based on real images, and synthetic ones is possible. We have functional tool for virtual experiments. Possible to discuss particular structures, also comparing of different structures on the basis of uniform criterion is available. One can give both examples in present work.

P-6: Automated Extraction of 3D Geometrical Features of Microstructure of Low Carbon Steel: *Yuki Arisato*[1]; Junya Inoue[1]; [1]The University of Tokyo

For structure-property relationships of materials, quantifying 3D microstructures is crucial, and serial sectioning has been widely utilized to construct the whole 3D microstructure. Usually, segmentation is applied to extract the shape and the distribution of individual microstructures. Supervised segmentation algorithms, in which all the microstructure is labeled beforehand, have been applied to 2D sectional images in most of the previous studies, but have a critical problem in the case of steel. That is, appearances of the microstructures, such as bainite and martensite, change drastically when their crystal orientations change, which make difficult for even an experienced researcher to identify the microstructures, and also increase drastically the number of training data set. In the present study, several unsupervised segmentation algorithms were applied to a 3D image of low carbon steel. Not only textural and statistical features in 2D sectional images but also 3D structural features were taken into account.

P-7: Characterization of Deformation Mechanisms in Polymer and Composite Materials Via Three Dimensional X-ray Imaging and Diffraction: *Maxime Pelerin*[1]; Henry Proudhon[1]; Lucien Laiarinandrasana[1]; Andrew King[2]; Jean-Paul Itié[2]; [1]MINES ParisTech - PSL Research University - Centre des Matériaux CNRS UMR 7633; [2]Synchrotron SOLEIL

PEKK (Poly-Ether-Ketone-Ketone) is a high-performance semi-crystalline polymer material developed by Arkema. The crystalline phase is crucial for maintaining mechanical strength with increasing temperature. Several key parameters such as degree of crystallinity and crystalline phase, polymer chain orientation, crystallite fragmentation, porosity... are determinant for mechanical properties and lifetime. The understanding of the evolution of these parameters during deformation is fundamental for better lifetime predictions and the design of polymers and polymer-based composites.We have used synchrotron tomography and diffraction techniques to study damage processes in PEKK and PEKK-based short carbon fibre composites during in situ mechanical testing. Phase Contrast Tomography (PCT) allows the study of porosity and cavitation once pores reach a sufficient size, but this corresponds to a very advanced state of damage. Prior microstructural changes could be revealed by diffraction, and two different approaches were tested to obtain spatially-resolved data: energy-dispersive diffraction and diffraction-tomography.

P-8: Combination of 3D and 2D Experimental Methods to Characterize Recrystallization Kinetics: *Dorte Jensen*[1]; Fengxiang Lin[2]; Yubin Zhang[1]; [1]Technical University of Denmark; [2]Universite Catholique de Louvain

The aim of this poster is to demonstrate how the understanding of recrystallization kinetics can be significantly improved by not only using one experimental technique (3D or 2D) but combining 3 complementary techniques. The 3 techniques are post mortem EBSP, in-situ 3DXRD and ex-situ SEM investigations and the material studied is 90% cold rolled copper. It is shown that the recrystallizing grains generally experience a fast growth to a limiting size, which is not due to impingements with other recrystallizing grains. The significant decrease in growth rates shortly after nucleation is shown to relate to a non-uniform migration behavior determined by the variations in the deformed microstructure. The implications of these results on the sample averaged kinetics and advancing recrystallization modelling are presented. The importance of combining the different experimental techniques is discussed and ideas for future 3D laboratory x-ray studies of recrystallization using LabDCT are finally presented

P-9: Development of a Solid Texture Synthesis Algorithm from Orthogonal 2D Exemplars: Tristan Ashton[1]; *Donna Guillen*[1]; William Harris[2]; Javier Morales[3]; [1]Idaho National Laboratory; [2]Massachusetts Institute of Technology; [3]University of Texas, San Antonio

The inverse problem of constructing 3D microstructures from 2D data is an area of active research within the materials science community. Fully deterministic volumetric reconstruction methods remain computationally expensive and relatively ill-defined. To circumvent these complications, we approach the problem from a statistical standpoint to reduce resource expenditure while maintaining reasonable fidelity to the source. We have implemented a computationally efficient algorithm in python using Fast Library for Approximate Nearest Neighbors (FLANN) to reconstruct the 3D features of interest in a given microstructure from three orthogonal 2D exemplars, benchmarked via histogram reweighting to avoid oversampling, and upsampling to preserve fine features. The algorithm is currently configured for two-phase materials and is being extended to accommodate multiple phases. Multithreading capability has been incorporated to provide a speedup of 80% over serial processing on a single compute node. The reconstructed microstructures are configured to ease of implementation in a finite-element method simulation.

P-10: Development of New High Energy Diffraction Microscopy Instrument at the Advanced Photon Source: *Robert Suter*[1]; Sangid Michael[2]; Ashley Spear[3]; Aaron Stebner[4]; [1]Carnegie Mellon University; [2]Purdue University; [3]University of Utah; [4]Colorado School of Mines

The U.S. National Science Foundation has funded a consortium based project (including the authors' institutions) to develop a new high throughput, high energy x-ray diffraction microscope (HEDM) instrument at the Advanced Photon Source (APS) at Argonne National Laboratory. The instrument should come on-line in 2019 and will be available to the general user community. It will be capable of near-field and far-field HEDM as well as computed tomography; sample environments will include room and high temperature (in gas atmospheres), and potentially other user developed compact systems. A significant effort will go into a tailored computing environment (in Python) that will control data collection and will stream data to computing resources for reduction of diffraction image sets to useful microscope outputs. This poster will describe the instrument development project.

P-11: Elastic Interaction between Twins during Tensile Deformation of Austenitic Stainless Steel: *Jette Oddershede*[1]; Nicolai Juul[2]; Grethe Winther[2]; [1]Xnovo Technology; [2]Technical University of Denmark

In austenite, the twin boundary normal is a common elastically stiff direction shared by the two twins, which may induce special interactions. This elastic interaction has been analysed and compared to grains separated by conventional grain boundaries. The 3D morphology of grains and twins in a 0.7x0.7x0.5 mm^3 316L austenite sample was measured in the undeformed state. The neighbour relations derived from this map were used to interpret the grain-averaged (Type-II) stress tensors measured after 0.12% tensile deformation at the Cornell High Energy Synchrotron Source.It was found that the components of the Type-II stress normal to the twin boundary plane exhibit the same large variations as for the conventional grain boundaries. Elastic grain interactions are therefore complex and must involve the entire set of neighbouring grains. The elastic-regime stress along the tensile direction qualitatively depends on the grain orientation, but grain-to-grain variations are large.

P-12: Feasibility Study of Dark-field Strain Microscopy: *Hanna Leemreize*[1]; Erik Knudsen[1]; Per Christensen[2]; Nikolaj Zangenberg[2]; Henning Poulsen[2]; [1]Technical University of Denmark; [2]Danish Technological Institute

Uncontrolled residual stresses in industrial devices can build up causing fatigue and failure. The formation and development of these stresses are poorly understood, in part because of the lack of efficient characterization techniques. A better understanding of these processes can elongate the life span of components, give more efficient component design and better materials properties. In this study, we prove the feasibility of a new technique that enables mapping of 3D strains within samples in a non-destructive and efficient manner.A combination of two optical components are used as a strain filter – a focusing lens with a slit system in its back focal point, BFP. By placing these in the diffracted beam, a direct image of the sample is formed with intensity in the regions where the given strain state is present. By scanning the slits in the BFP we can now map the strain in a tomographic manner.

P-13: Large 3D-EBSD Dataset Acquisition for Stochastic Modeling of Microstructures by Random Marked Tessellations: *Jaromír Kopecek*[1]; Jarmila Remiášová[1]; Ladislav Klimša[1]; Jakub Stanek[2]; Viktor Beneš[2]; Lucas Petrich[3]; Daniel Westhoff[3]; Carl Krill[3]; Volker Schmidt[3]; [1]Institute of Physics of CAS; [2]Charles University; [3]Ulm University

Random marked tessellation models have proven their usefulness in gaining deeper understanding of polycrystalline microstructures, which are important to processes like grain growth. However, the formulation of physically relevant tessellation models relies on the availability of highly resolved 3D data sets acquired from real materials. To this end, we have utilized 3D-EBSD to characterize samples of the superplastic aluminum alloy Al-3Mg-0.2Sc, which were subjected to 4 or 8 passes of equal channel angular pressing (ECAP) in order to obtain grains small enough for conventional 3D-EBSD with a Ga focused ion beam

(FIB). For purposes of comparison, Xe-plasma FIB milling was also carried out on these specimens, which enlarged the scanned volume by an order of magnitude. The data from both devices—FEI Quanta and TESCAN FERA3—were processed and analyzed using the software package DREAM.3D. The resulting reconstructions serve as the basis for identifying random marked tessellation models that are suitable for representing the sample microstructures.

P-14: Manufacture of Rubber Asphalt Mixtures with Local Materials: Guilliana Agudelo[1]; [1]Universidad de Antioquia

This work shows the results of mixing asphalt 60/70 with wet rubber powder. Rubber is a by-product of recycled tires in Colombia. The main objectives are to reduce the negative impact of discarded tires in the city and manufacture a competitive asphalt with this material. A total of 15 mixtures with rubber contents ranging from 10 to 20% were prepared. The characterization of the materials involved is presented (microstructural and chemical) by optical and electronic microscopy techniques; and chemical composition tests. In addition, various mechanical and performance tests are included on the samples made. This work has a potential great environmental and economic impact in Colombia.

P-15: Modeling and Analyzing the Microstructure Evolution of SOFC Anodes During Operation: *Matthias Wieler*[1]; Patricia Haremski[1]; Paul Hoffrogge[2]; Daniel Schneider[2]; Britta Nestler[2]; Florian Wankmüller[3]; André Weber[3]; Matthias Meffert[3]; Heike Störmer[3]; Thorsten Dickel[4]; Piero Lupetin[1]; [1]Robert Bosch GmbH; [2]Hochschule Karlsruhe; [3]Karlsruhe Institute of Technology; [4]RJL Micro & Analytic GmbH

An important degradation mechanism in solid oxide fuel cells (SOFCs) is the microstructural evolution of Ni-YSZ anodes under operating conditions caused by diffusional transport of nickel. In this work, we combine experiments and simulations in order to investigate and model these microstructural changes in a novel full-ceramic co-sintered SOFC. Goal of the study is to develop a phase-field model that incorporates all transport mechanisms relevant for anode degradation: volume diffusion, interface diffusion, and grain boundary movement. The material parameters required for the model are determined via thermal grooving experiments on bicrystalline and polycrystalline nickel. To obtain the initial microstructure for the simulation and to validate the simulation results, we analyze the 3D microstructure of newly fabricated and aged specimens with FIB-SEM, nano-CT, and EBSD-EDXS. Finally, the impact of anode degradation on the performance of the SOFC is evaluated.

P-16: Real-time Synchrotron Imaging of Silicic Magma Degassing: Insights into Bubble Nucleation and Growth Kinetics during Controlled Heating: *Rafael Torres-Orozco*[1]; Nolwenn Le Gall[1]; Mathew Pankhurst[1]; Biao Cai[1]; Robert Atwood[2]; Sara Nonni[1]; Peter Lee[1]; [1]Manchester X-ray Imaging Facility; [2]Diamond Light Source

Synchrotron x-ray imaging has enhanced the understanding of magma degassing processes. Here, we present novel, time-resolved (4D) synchrotron microtomography (I12 beamline, Diamond Light Source, UK) of vesiculation in water-bearing (<1 wt.%) silicic melts, under isothermal and non-isothermal during heating (from 850 to 1250 °C) at constant rate (0.4 or 0.1 °C s-1) and ambient pressure. Preliminary observations suggest that bubble nucleation is typically delayed until high temperatures prompt lower melt viscosity. Nucleation is followed by rapid bubble growth, bubble coalescence, and the formation of permeable channels in the inner part of the samples due to water diffusion outside of the melt. This morphology of permeable foam facilities outgassing, and has previously been associated with effusive and/or low explosive volcanic eruptions. These observations provide a pathway for future step-change 4D experiments under controlled pressures, elucidating degassing phenomena, crucial for understanding eruptive styles and intensities during eruptions of different magnitude and composition.

P-17: Single Grain Characterisation at the HEMS-Beamline: *Torben Fischer*[1]; Lars Lottermoser[1]; Norbert Schell[1]; Peter Staron[1]; Martin Müller[1]; [1]Helmholtz-Zentrum Geesthacht

The 3D investigation of polycrystalline materials allows the study of the relationship between macroscopic and micro structural properties at the level of single grains. A main objective is the measurement of the grain boundary topology, orientation gradients, and 3D strain state between single grains during deformation. The High Energy Materials Science Beamline (HEMS), operated by the Helmholtz-Zentrum Geesthacht (HZG), has a dedicated hutch for such 3D techniques. HEMS is situated at synchrotron storage ring PETRA III at DESY and has a tuneable energy range between 35 and 200 keV. The main scientific topics addressed are the investigation of new processes, metallurgy, chemistry and material physics. The grain mapper is an dedicated endstation for the 3D-XRD technique. Fast detector systems and high photon flux allow for highly dynamic investigations, e.g. of phase transformation or catalysis. The instrument is now in user operation. First results of material science experiments will be shown.

P-18: The Dark-field X-ray Microscope at ID06: *Carsten Detlefs*[1]; [1]ESRF

We present a new instrument for dark-field x-ray microscopy installed on beamline ID06 of the ESRF. Dark-field x-ray microscopy is a new way of three-dimensionally (3D) mapping lattice strain and orientation in crystalline matter. It is analogous to dark-field electron microscopy in that an objective lens magnifies diffracting features of the sample. The use of high-energy synchrotron x-rays, however, means that these features can be large and deeply embedded. The spatial and angular resolution can reach 100 nm and 0.001°, respectively. The instrument furthermore allows pre-characterization of samples at larger length scales using 3DXRD or DCT, such that a region of interest such as a single grain can be selected for high-resolution studies without the need to dismount the sample. This ability to directly characterize complex, multi-scale phenomena in situ is a key step towards formulating and validating multi-scale models that account for the entire heterogeneity of materials.

P-19: The Effect of Surface Roughness on the Fatigue Life of Additively Manufactured Ti-6Al-4V Components: Gregory Lamb[1]; *Oluwatobi Kalejaiye*[1]; Cynthia Waters[1]; [1]North Carolina A&T State University

Additive Manufacturing (AM) is becoming one of the most influential manufacturing technologies of the 21st century, with its capabilities of rapid prototyping and design versatility sweeping the industry by storm. Despite this, a major hindrance to the technology is part validation, as material properties are machine specific. Most AM processes use a layer-by-layer buildup of material to manufacture components, causing the outermost layer to remain in sintered powder form. This phenomenon causes poor surface finishing, adding surface roughness as a function of the powder size used. The purpose of our research is determining the effects this surface roughness has on the fatigue life of a ASTM E466-15 derived Ti-6Al-4V fatigue test specimen. Using the fatigue testing capabilities of Abaqus, we will model conditions and surface finishes from various machines; gaining valuable insights into the characterization of these variables and how to use them to validate AM components in the industry.

P-20: The Synthesis and Characterization of Ca and Al Doped Lanthanum Manganite Coated Porous SiC Foams for Syngas Production Processes: *Mohammad Saadatfar*[1]; Amir Masoud Parvanian[2]; Hamidreza Salimijazi[2]; [1]Australian National University; [2]Isfahan University of Technology

Solar assisted hydrocarbon fuel production through the conversion of CO2-H2O mixture to CO-H2, a process known as syngas fuel production is a promising method of renewable energy production and supply. Materials such as Calcium and Aluminum doped lanthanum manganite (LCMA) have shown a great yield of conversion in syngas production processes. We combine high thermo-chemical conversion efficiency of LCMA with excellent mass and heat transfer capabilities of porous ceramics to increase the overall conversion efficiency. Characterization of pore morphology and coating homogeneity on the porous networks were performed using an x-ray computed tomography techniques. Our results show a strong dependency of coating thickness and homogeneity with the intrinsic properties of the porous network. We show that wider pore size distribution and the presence of larger pores result in a more effective coating and better connectedness of the coated layer, which in turn result in higher performance of surface-based catalytic processes.

P-21: Three-dimensional Structure of Deformation Twins in Magnesium: *Todd Hufnagel*[1]; Hao Sheng[1]; Ravi Shivaraman[1]; Vignesh Kannan[1]; K. T. Ramesh[1]; [1]Johns Hopkins University

Twinning is an important mechanism of plastic deformation in magnesium and similar hcp metals that have a limited number of easy slip systems. Understanding the nucleation and growth of twins, as well as how they interact with each other and with other microstructural features such as grain boundaries, is therefore important for the development of new alloys with improved mechanical properties. The assessment of twin-twin interactions, in particular, is important for plasticity models that address hardening mechanisms. Because traditional approaches to characterization provide only limited information about the three-dimensional twin structure, we have used 3D EBSD serial sectioning (performed in the SEM chamber with a fs pulsed laser) to study deformation twins in magnesium produced by dynamic deformation at rates of ~1000 1/s. We compare the results with traditional (2D) characterization, and also discuss the effect of laser-material interactions on the twin microstructure.

P-22: 3D Characteristics of Porosity in Additive-manufactured Titanium Alloys and Their Influence on Mechanical Properties: *Shao-Gang Wang*[1]; Lei Zhang[1]; [1]Institute of Metal Research, Chinese Academy of Sciences

Additive Manufacturing techniques such as selective laser melting (SLM) and electron beam melting (EBM) could build titanium components for medical and aerospace applications. In this work, full dense Ti–6Al–4V samples were fabricated by using EBM and SLM. 3D X-ray tomography (XRT) technique was employed to find 3D features of defects as pore distribution difference etc. Varied mechanism of defect formation was proposed. Unexpected 3D characteristics were also revealed and their influence on tensile strength and fatigue property were compared. In comparison with full dense Ti–6Al–4V alloys, porous structures of Ti2448 produced by EBM and SLM were also investigated. The effect of pore features on compression and fatigue properties were discussed. Tuning scan speed of heating source beams affected the porosity as size and amount, which influence the stress response of porous Ti2448.

P-23: 3D Dislocation Structure in Proton Irradiated Singe Grains of Polycrystalline Zirconium: Matthew Topping[1]; Gyula Zilahi[2]; Sandeep Irukuvarghula[1]; Gábor Ribárik[2]; Alistair Garner[1]; Peter Kenesei[3]; Philipp Frankel[1]; Michael Preuss[1]; *Tamás Ungár*[1]; [1]Materials Performance Centre, The University of Manchester; [2]Eötvös University Budapest; [3]Argonne National Laboratory

Integrity of fuel cladding Zr structures is a key issue in power generating nuclear reactors. Long term radioactivity makes it difficult to determine irradiation induced damage in neutron irradiated Zr. Short-lived activation and similar damage structure make proton irradiated Zr excellent surrogates for neutron irradiated Zr. Irradiation in Zr alloys produces dislocation loops, characterized by electron microscopy or X-ray diffraction. X-ray powder diffraction proves to be a powerful method to characterize average properties of dislocation loops. However, proton irradiation, unlike neutron irradiation, is unidirectional due to the beam line. Therefore, the inherent anisotropy of hcp Zr raises the question to what extent grain orientation and depth influences the grain-to-grain dislocation structure in proton irradiated Zr. We will show that 3D high angular resolution single grain diffraction experiments carried out at the 1-ID beamline of APS synchrotron at ANL can help concluding about similarities and differences between neutron and proton irradiation.

P-24: 3D Intergranular Crack Growth Modeling in Ceramics: *Emile Renner*[1]; François Guillet[1]; Rafael Estevez[2]; Cristian Ovalle[2]; [1]CEA Le Ripault; [2]Grenoble Alpes University

Ceramics are brittle materials where the most critical default drives the cracks initiation. Some ceramics are prone to slow crack growth (SCG) which leads to failure at load levels lower than their critical toughness. Experimental tests can be conducted on polycrystalline samples in various conditions to study how SCG kinetics affects toughness. However, it is complicated to take into account all aspects of a given ceramic to predict its lifetime, especially for complex loading and geometries. Thus, we propose a 3D finite element model (FEM) of the material microstructure representative elementary volume, considering the SCG kinetics. The polycrystalline microstructure model must respect the porosity and the grain size distribution. A 3D cohesive zone model for intergranular SCG is developed at the SIMaP laboratory. The fracture is then studied through mechanical tests as uniaxial tensile, 4 points bending and double-torsion, built using FEM and simulation results are confronted with experimental ones.

P-25: 3D X-ray Diffraction Microscopy (3DXRD) Using High Resolution X-ray Nanodiffraction: *Hergen Stieglitz*[1]; Christina Krywka[1]; Martin Müller[1]; [1]Helmholtz-Zentrum Geesthacht

The existing technology called 3DXRD, is a well-established technique to map the grain structure of polycrystalline systems. Due to a given beamsize and limits of the reconstruction software only a few grains can be tracked, resulting in a minimum mappable grainsize. The planned experiment shall utilize a nano-focused synchrotron beam (e.g. Nanofocus Endstation of P03, PETRA III) to examine very fine-grained systems. With respect to the small beamsize of about 100 nm cross section, the precise positioning of the sample becomes more important to secure grains to be in a constant scanned volume to avoid mistakes while reconstructing. To meet this challenge a stable and wobble-free rotary stage is planned to ensure a constant gauge volume. We want to use an interferomenter-based feedback loop to compensate the runout of the sample with a XY-stage. A further step is the adjustment of the software for the needs of a nano-focused beam.

P-26: 4D X-ray Tomography Investigation of Dendrite Evolution in Al Alloys: *Tiberiu Stan*[1]; Yue Sun[1]; Kate Elder[1]; Xianghui Xiao[2]; Michel Rappaz[3]; Peter Voorhees[1]; [1]Northwestern University; [2]Argonne National Laboratory; [3]Ecole Polytechnique Federale de Lausanne

The mechanisms by which metallic dendrites grow remain controversial and not well understood. The 4D evolution of dendritic two-phase mixtures in Al-Cu and Al-Zn alloys is determined using coupled in-situ x-ray computed tomography (XCT) and x-ray diffraction (XRD). The experiments give new information about: solid-liquid volume fractions, dendrite tip growth rates and morphologies, secondary branch spacings and symmetries, interfacial curvatures and areas, and coarsening dynamics. Conventional Al – 20 wt% Zn alloys solidify via fcc Al dendrites which grow in <100> directions. The addition of just 0.1 wt% Cr leads to twinned dendrites which instead grow in <110> directions. It is postulated that the Cr addition forms metastable five-fold symmetric quasicrystals with edges that favor the nucleation of twinned dendrites. The combination of 4D XCT and XRD techniques used in this study provide new insights into the growth of regular and twinned dendrites in metallic alloys.

P-27: A 3D Coupled Approach for Fatigue Life Prediction of Titanium Aluminides: Fom Experimental Observations to Polycrystalline Calculation: *Louise Toualbi*[1]; Pierre Serrano[1]; Pascale Kanoute[1]; Alain Couret[2]; [1]ONERA - The French Aerospace Lab; [2]CNRS

Deformation of TiAl alloys is strongly influenced by local microstructure, which can lead to non-negligible strain localizations. In this paper we propose an approach combining in-situ tensile tests, 3D-reconstructed microstructure and calculation on polycrystals. The aim of this work is to assess the model response in terms of slip activity and stress concentration. A Digital Image Correlation analysis is performed on in-situ tensile tests to measure local strain fields. The cyclic behaviour of various microstructures, characterized by grain size, volume fraction and lamellae size, is studied. In parallel, a polycrystalline calculation constructed within a crystal plasticity framework is developed. Correlation with experimental data is made using 3D-reconstruction from EBSD maps. The results obtained at this scale are compared to the macroscopic response given by the multiscale constitutive behavior model developed at the ONERA. These results are used to propose a microstructure sensitive fatigue model for TiAl alloys.

P-28: Advanced FIB-SEM Tomography Including 3D Analytics like EDS and EBSD: *Tobias Volkenandt*[1]; Fabián Pérez-Willard[1]; Michael Rauscher[1]; [1]Carl Zeiss Microscopy GmbH

Material characterization studies often require 3D investigations at high resolution in all three dimensions. FIB-SEM tomography is a well-established technique to provide this. Especially since it can be combined with analytical techniques like EDS or EBSD to provide not only visual but also analytical information about the volume of interest. However, until now there has been a gap between the ideal imaging conditions and those ideal for the analytic mapping. We will present latest improvements to our advanced FIB-SEM workflow that allow automated switching of working conditions (such as acceleration voltage or beam current) during the acquisition. This leads to image stacks of best resolution in all dimensions together with 3D analytical data of highest quality. Exemplary results obtained from different types of samples will illustrate the workflow and prove that it is no longer necessary to sacrifice SEM resolution when adding analytics to a FIB-SEM tomography.

P-29: Advances in 3D Correlative Multiscale Tomography: *Bartlomiej Winiarski*[1]; Grzegorz Pyka[1]; Austin Wade[2]; Ali Chirazi[1]; Daniel Lichau[1]; Grace Burke[2]; Philip Withers[2]; [1]Thermo Fisher Scientific; [2]University of Manchester

Three-dimensional correlative multiscale multimodal microscopy, also known as correlative multiscale tomography, is a dynamically developing complex materials science and life science research platform. It's modular design incorporates six major routines: a) instrumentation/experimental and sample preparation techniques, b) digital 3D data recording and storage, c) processing, coregistraction and segmentation, d) visualization of 3D micro structures, e) analysis and quantification and f) virtual 3D simulation and testing.In this contribution we demonstrated advances in the 3D correlative microscopy accelerated with latest HeliScanTM micro CT system, Helios™ PFIB–SEM DualBeam™ microscope and unique, software integrated instrumental environment using inter-linked software: Auto Slice&View 4™, Avizo™, iFAST™, Maps™ and AutoScript™. As practical examples we investigated micro-structural imperfections, cracks and local residual stresses developed in additively manufactured IN718 sample via blown powder direct laser deposition. The combined capabilities of hardware and software allowed obtaining a new insight into manufacturing defects developed during direct laser deposition.

P-30: Analysis of Thermal and Mechanical Responses of Porous Materials: *Jaehyung Cho*[1]; Geon Young Lee[1]; Kyu Jung Yeom[1]; Jong Joo Rha[1]; [1]Korea Institute of Materials Science

Microstructure with various pore structures was modeled using 3-dimensional CAD and its thermal and mechanical responses were analyzed using FE analysis. Various factors such as porosity, pore shape and its spatial distributions were considered to investigate thermal and mechanical responses. Overall, thermal conductivity decreased with increase in porosity. Elastic modulus also decreased with porosity. Anisotropic distribution of pore structure affected thermal and mechanical responses.

P-31: Assessment of Hydrogen Embrittlement through 3D Strain Visualization in Aluminum Alloys: *Hang Su*[1]; Kazuyuki Shimizu[1]; Md. Shahnewaz Bhuiyan[1]; Hiroyuki Toda[1]; Kentaro Uesugi[2]; Akihisa Takeuchi[2]; Yoshio Watanabe[3]; [1]Kyushu University; [2]JASRI; [3]UACJ Corporation

Microstructural features tracking and related 3D strain visualization techniques are useful to understand the relationships between microstructures and localized heterogeneous deformation inside material. Hydrogen induced localized strain concentration, as well as the initiation and propagation of hydrogen induced quasi-cleavage crack in the strain localization region are discussed through measuring 3D strain distribution at low applied strain levels. By applying hydrogen trapping analysis, effects of hydrogen trap sites such as dislocations, nano voids and intermetallic particles on the hydrogen migration, accumulation and partitioning behaviors in the strain localization region are studied. It has been confirmed that 3D strain visualization technique and hydrogen trapping analysis make visualization of localized hydrogen partitioning possible in three dimensions in aluminum alloys.

P-32: Characterization of Powder Al Alloys and the Effects of Thermal Processing, in Three Dimension: *Caitlin Walde*[1]; Danielle Cote[1]; Richard Sisson[1]; Victor Champagne[2]; [1]WPI; [2]US Army Research Laboratory

Gas-atomized metallic powders are commonly used in solid-state additive manufacturing processes. While their post-process consolidated properties are widely studied, there is little research on the properties of the powders before consolidation. Understanding the powder characteristics before use in additive manufacturing could lead to fine-tuning properties of additively manufactured materials. As powder properties and characteristics differ greatly from their wrought counterparts, it is important to fully understand the unique structure of these powders. This research characterizes three-dimensionally the grain structure and secondary phases of aluminum alloy powders after various thermal processes. This is accomplished through the use of a serial sectioning technique that combines SEM images and EBSD results of numerous planes throughout the powder particles. Secondary phases are further analyzed using TEM/STEM and DSC.

P-33: Characterization of Three Dimensional Transport Networks in a Long-Term Tested Solid Oxide Electrolysis Cell: *Peter Stanley Jørgensen*[1]; Jacob R. Bowen[1]; Ming Chen[1]; [1]Technical University of Denmark

Solid oxide electrolysis cell (SOEC) is a promising technology for energy conversion and storage. The SOEC cell consists of two electrodes on each side of a dense electrolyte. The electrodes are typically a two- or three-phase porous system, where the solid phases are responsible for conduction of electrons and oxygen ions and the pore phase allows transport of reactants and products to and from the electrochemically active sites. In this work we present a study of three dimensional transport networks in a long-term tested SOEC. The difference in the transport network quality at different cell locations was compared in terms of 3D microstructure parameters calculated from FIB serial sectioning image data. An advanced 3D transport network analysis was performed through simulations and geometrical calculations. Dramatic differences were observed between the gas inlet and outlet in the cell. The obtained 3D transport characteristics correlated well with the measured cell electrochemical performance.

P-34: Characterizing Structure-property Relationships in Aluminum-carbon Hybrid Materials: *Christopher Shumeyko*[1]; Daniel Cole[1]; Xiaoxiao Ge[2]; Lourdes Salamanca-Riba[2]; [1]US Army Research Laboratory; [2]University of Maryland

A class of metal-carbon hybrid materials deemed covetics, have exhibited advantageous mechanical, thermal, and electrical properties in recent years. While this class of materials have promising applications ranging from the aerospace industry to power transmission, there remain great gaps in their process-structure-property relationships. In this work, we utilize molecular dynamics simulations and nanoindentation experiments to elucidate the effect of microstructure on the mechanical response of aluminum covetic materials. Specifically, the role and properties of Al-C interfaces are investigated, including the nature of bonding which give covetic materials superior thermodynamic stability. Materials characterization through EELS, Raman Spectroscopy, TEM, and XPS provides a framework for computational models, while simulations aim to guide future processing techniques for scalability and stability of covetics.

P-35: Characterizing Voids During Ductile Fracture of a Dual Phase Steel Using X-ray Computed Tomography and Xe+ FIB Serial Sectioning EBSD: *Yi Guo*[1]; Timothy Burnett[1]; Kyono Hirofumi[2]; Hirofumi Ohtsubo[2]; Kaoru Sato[2]; Philip Withers[1]; [1]Henry Moseley X-ray Imaging Facility; [2]JFE Steel

We demonstrate a correlative approach to study voids, formed during ductile fracture of a Ferritic-Bainitic steel, using a combination of time-lapse X-ray computed tomography (CT) and serial sectioning EBSD (SSE). The X-ray tomography followed the nucleation and growth of voids during deformation and provides statistical information regarding the distribution and volume fraction of voids at micrometre length scale. The SSE enables a site specific excavation of a relevant volume, guided by the CT results, and provides information on the grain neighbourhoods around these voids in 3D with details on a finer length scale. With this approach, features of interest can be targeted and purposely studied. Both spherical and ellipsoidal voids were characterised focusing on the grain orientations and patterns of deformations in 3D around the voids, with Schmid factor calculations on the full 3D grain orientations to understand the deformations leading the observed shape difference.

P-36: Coherent X-ray Diffractive Imaging Simulated by Monte Carlo Ray-tracing: *Giovanni Fevola*[1]; Erik Bergbäck Knudsen[1]; Tiago Ramos[1]; Gerardina Carbone[2]; Jens Wenzel Andreasen[1]; [1]Technical University of Denmark; [2]MAX IV

Coherent diffractive imaging (CDI) techniques have gained significant momentum in recent years, and most synchrotrons have dedicated beamlines for CDI techniques, with full-field CDI and ptychography (near-field and far-field) among the most commonly applied. Tomographic ptychography combines a large field of view with the capability to image structures in 3D down to about 10 nm in resolution. Simulations of CDI experiments can assist in interpretation of data by regularization of 3D reconstruction to help distinguish signal from noise, or to design experiments that minimize X-ray dose. Several factors are however hampering simulations in a ray-tracing framework, and so far only simplified test-cases have been reported. In this talk, we detail novel enhanced CDI features of the ray-tracing software McXtrace[*], and discuss their ability to produce ptychographical datasets. References: [*] E. Bergbäck Knudsen et al., J. Appl. Crystallogr. 46, 679–696 (2013).

P-37: Comparison of Strains Calculated by Crystal Plasticity FE Models Based on the Microstructure Measured by 2D EBSD and 3D EBSD-FIB Techniques and with those Measured by Means of DIC: *Markus Niffenegger*[1]; Vicente Herrera-Solaz[1]; Maria Pérez-Prado[2]; Luca Patriarca[3]; Carmen Capeda[4]; Javier Segurado[4]; [1]Paul Scherrer Institut; [2]IMDEA Material Institut; [3]Politecnico di Milano; [4]IMDEA Materiales

Crack initiation and growth of micro-cracks due to high cycle fatigue (HCF) require the consideration of the microstructure. In the present work, the microstructure of the austenitic stainless steels 316L has been mapped by means of 2D and 3D EBSD-FIB techniques. The orientation maps (grain geometry and orientation) have been successively used to build the corresponding 3D finite element (FE) models. The material behavior is taken into account by Crystal Plasticity code (CAPSUL) and by a simplified in-house code (SNF) for HCF estimation, which simplifies the material behavior and optimizes the computational cost. The question, whether pseudo 3D FE models based on 2D EBSD measurements are sufficient to estimate stresses, strains and HCF lifetime is discussed. Furthermore, preliminary conclusions about the strain fields in a pseudo 3D FE model calculated by means of the CAPSUL and SNF and those measured by Digital Image Correlation (DIC), will be drawn.

P-38: Data-driven Modeling of Microstructure Shape Influence on High Cycle Fatigue Life of NiTi Wire: *Orion Kafka*[1]; Cheng Yu[1]; Modesar Shakoor[1]; Wing Kam Liu[1]; [1]Northwestern University

Nickel-titanium arterial stents and heart valve frames must withstand on the order of one billion heart beats, which results in predominantly axial cyclic loading in the struts of the device. The conventional wire-drawing process induces inclusion break-up, "stringers," which reduces inclusion axial cross-sectional area while increasing the transverse area. We investigate the influence of final stringer geometry – shape and size of inclusion and voids resulting from inclusion break-up – on fatigue crack incubation life using a fast computational method called crystal plasticity self-consistent clustering analysis. This recently developed method, based data-driven modeling techniques, solves the crystal plasticity constitutive equations within a periodic, 3D representative unit cell. The efficiency of the method allows for parametric study of simplified stringer-like geometries and imaged 3D geometry obtained with serial-sectioning or x-ray tomography. This information can be used for material and manufacturing design, e.g. by providing a design goal that allows for optimization.

P-39: Effect of Powder Recycling and HIP-treatment Improvement on Titanium Parts Manufactured by Arcam EBM: *Vladimir Popov*[1]; Alexander Katz-Demyanetz[1]; Andrey Garkun[1]; Gary Muller[1]; Evgeny Strokin[1]; [1]Technion - Israel Institute of Technology

Electron beam melting (EBM) is a well-known effective manufacturing process. However, the priority of proper non-porosity microstructure and relevant mechanical properties is still a challenge for main applications of Titanium Additive Manufacturing including EBM, such as airspace industry and medical implants production. Thus, quality of the powder and standardization of the AM process come to the front. The influence of Ti-6Al-4V powder recycling, the reasonable number of cycles, the requirements to recycling procedures, possible post processing procedures – are still open issues. Aiming to answer these questions, we evaluate two same cylinder sets, printed one from recycled powder and another from the new powder batch. Moreover, the effect of Hot Isostatic Pressure (HIP) treatment was investigated, to clarify the possibilities of this treatment to improve microstructure and mechanical properties of the parts manufactured from highly re-used powder.Samples from the new and re-used powder were examined before and after HIP.

P-40: Elastic Grain Interactions in a Polycrystalline Wire Analyzed by a Numerical Model Reconstructed from 3D-XRD Data: *Ludek Heller*[1]; P. Shayanfard[1]; R. Quey[2]; P. Sittner[1]; I. Karafiatova[3]; Z. Pawlas[3]; [1]Czech Academy of Sciences; [2]IMT Mines Saint-Etienne; [3]Charles University

In this work, we analyze inter/intra-granular stress fields created during elastic deformation of elastically anisotropic NiTi wire subjected to uniaxial tensile loading. The analysis is based on finite element (FE) simulations using a model of the polycrystalline wire reconstructed from 3D-XRD data, consisting of the grain centroids, volumes, and orientations. A FE model of ~2500 grains is reconstructed using a new dedicated technique based on the optimization of Laguerre tessellation. The inter/intra-granular stress fields are calculated by subjecting the FE model to the same uniaxial force as that used in the 3D-XRD experiment. In order to find out whether the simulated stress fields are realistic, the simulated grain-averaged values of the grain stresses are compared with their experimental 3D-XRD counterparts. Furthermore, the simulated inter/intra-granular stresses are statistically correlated to lattice orientations of individual grains, as well as to the mismatch in microstructural attributes of neighboring grains (lattice misorientations, volumes' difference).

P-41: High Energy X-ray Diffraction at CHESS-U: *Matthew Miller*[1]; [1]Cornell University

The use of high energy x-ray diffraction (HEXD) methods, which includes 3DXRD, HEDM and DCT, has experienced unprecedented growth at high energy synchrotrons around the world. Over the past several years, HEXD at the Cornell High Energy Synchrotron Source (CHESS) has been used to examine a wide spectrum of processes such as fatigue crack growth in aluminum, high rate phase transformations in steel and fatigue crack initiation in copper. CHESS is undergoing a major upgrade (CHESS-U), new experimental stations will be created. A new high energy beamline will focus specifically on capturing diffraction data during processing operations and will employ synchronous data reduction; users should expect to leave with real materials data not just x-ray images. This talk will describe the ongoing HEXD experiments and capabilities at CHESS and the attributes of the new high energy CHESS-U beamline.

P-42: In-situ Synchrotron X-ray Diffraction and Digital Image Correlation Study on Stress-induced Martensitic Transformation of a NiTi Subjected to Monotonic Uniaxial Tension: *Xiaohui Bian*[1]; Ahmed Saleh[1]; Peter Lynch[2]; Azdiar Gazder[1]; Christopher Davies[3]; Elena Pereloma[1]; [1]University of Wollongong; [2]Deakin University; [3]Monash University

In-situ monotonic uniaxial tensile test using synchrotron X-ray diffraction and digital image correlation were conducted on a superelastic NiTi. The diffraction data from the sample centre over the tensile test was collected. In addition, the diffraction data along the gauge length at five selected strains was acquired. In this way, the localised stress-induced austenite-martensite transformation can be visualised from both macroscopic and microscopic views. During localisation the specimen is divided into untransformed region, transformed region, and transformation band front (with both phases). The lattice strain, peak width of individual grain families, phase volume fractions and stress-induced martensitic texture, and strain fields, strain rate distributions were studied. These parameters keep unchanged in the untransformed and transformed regions, whereas they vary within the narrow transformation front. Therefore, the strain state and loading partitioning in (retained) austenite and martensite within the transformation front, and their relation to the transformation mechanism are discussed.

P-43: Integral Mean Curvature Analysis of Normal Grain Growth Using Diffraction Contrast Tomography: Catherine Sahi[1]; *Jun Sun*[2]; Allan Lyckegaard[2]; Burton Patterson[1]; Yubin Zhang[3]; Florian Bachman[2]; Nicolas Gueninchault[2]; Hrishikesh Bale[4]; Dorte Juul Jensen[3]; Robert DeHoff[1]; [1]University of Florida; [2]Xnovo Technology; [3]Technical University of Denmark; [4]Carl Zeiss X-ray Microscopy Inc.

The growth rate of individual grains of Armco iron was found to be linearly related to their integral mean curvature Ms as predicted by the recent DeHoff model, with zero curvature near 14 faces. Growth rates were determined by comparison of individual grain volumes over incremental anneal times and their Ms values determined by the innie-outtie technique performed on voxelated 3D images. The 3D images for these measurements were obtained by laboratory diffraction contrast tomography (LabDCT) analysis. In a related study of Ms during particle pinning, the boundary curvature was monitored before, throughout particle interaction and breakaway and after static pinning. Evolution of the measured curvature was observed as the boundary evolved through a range of complex shapes to maintain the necessary contact angle with the particle. The little-noted fact that the average boundary curvature, i.e., the driving force for motion, approaches zero at static pinning was observed.

P-44: Investigation of the 3D Microstructure of Additively Manufactured 316L Stainless Steel: *Lily Nguyen*[1]; David Rowenhorst[2]; Richard Fonda[2]; [1]National Research Council / Naval Research Laboratory; [2]Naval Research Laboratory

Additive manufacturing (AM) is a layer-by-layer processing technique that results in a highly complex microstructure. Due to the inherent 3D nature of this process, 2D observations provide an incomplete understanding of how its microstructure forms. This presentation will describe how a fully automated serial sectioning system was developed to collect a large volume of AM 316L using traditional SEM imaging and EBSD data at a high resolution. We will also present an initial analysis that shows the scan strategies, including build direction and scanning direction, can affect the crystallographic texture and morphology of the grains. We will present our results using spatial and texture analysis to examine the relationship between microstructure and AM processing.

P-45: Large Volume 3D Characterization of Graphite Microstructures in Nodular Cast Iron by Plasma FIB: Juan Carlos Hernando[1]; Doru Michael Stefanescu[2]; *Ehsan Ghassemali*[1]; Jirí Dluhoš[3]; Hana Tesarová[4]; Martin Sláma[4]; Attila Diószegi[1]; [1]Jönköping University; [2]Ohio State University and University of Alabama; [3]TESCAN ORSAY HOLDING, s.r.o., Czech Republic; [4]TESCAN ORSAY HOLDING, a.s., Czech Republic

Material properties in cast components are principally determined by the microstructures developed during the solidification process. The complexity of these microstructures made 3D tools indispensable for an accurate characterization and analysis of these phases. Cast iron microstructures usually exceed the size suitable for a 3D analysis within a reasonable time and a fine resolution, making the use of the current 3D techniques scarce in the literature of this material. In this work, the application of Xe-Ion plasma focused ion beam (FIB) tomography to large volumes up to 200 µm3, provided information of the spatial arrangement and internal structure of the graphite nodules. The 3D analysis revealed the presence of Fe-rich inclusions embedded within the radial carbon sections of the nodule, suggesting different growth mechanisms during the solidification. These results confirm the existence of three different graphite nodules populations in nodular cast iron, as suggested in recent literature using 2D investigations.

P-46: Lattice Structure Optimization for Thermal Insulation: From Design to Multi-scale Characterization: *Sylvain Chupin*[1]; Yohann Scaringella - Guerritat[1]; [1]CEA

Super-insulating materials (material with better thermal properties than air) are mechanically very fragile. Generally, the insulating part of the material is made by a nanoporous silica matrix (extremely low mechanical strength) and the mechanical structure is insured by glass fibers dispersed within this matrix. The goal of our study is to replace the glass fibers by an optimal structure that gives a better mechanical behavior without degrading the thermal properties. To reach this goal, topological optimization is used to find the lattice structure giving the best thermal and mechanical compromise. These structures are made using the stereolithography additive manufacturing process.Therefore, the results are highly dependant of the local properties of the solid elements. Multi-scale characterizations are made from the lattice element (~50 µm) to the material (~2 mm). This experiments are used to understand process/properties relations and to improve the optimization structure generation.

P-47: Local 3D Fiber Orientation Analysis for Fiber Reinforced Composite Materials: *Dascha Dobrovolskij*[1]; Katja Schladitz[1]; [1]Fraunhofer ITWM

Glass fiber reinforced composite materials are popular due to their light weight advantages. These composite materials are frequently used in various applications. A proper design of technical components requires the entire knowledge about the material microstructure. We present here recent image processing results regarding the fiber orientation estimation in 3D images acquired by X-ray computed tomography. State-of-the-art methods for gray value based orientation estimation do not require single fiber segmentation. It was shown, that methods based on first or second order gray value derivatives are reliable and robust w.r.t. noise. Here, we report on additional experiments to evaluate the influence of the resolution, the fiber volume fraction, and the preprocessing on the quality of the orientation estimation. Moreover, the influence of the averaging for computing second order orientation tensors isexamined, too.

P-48: Local Thermal Residual Elastic Strains in Ductile Cast Iron Measured Using Synchrotron X-ray Microdiffraction: *Yubin Zhang*[1]; Tito Andriollo[1]; Søren Fæster[1]; Ruqing Xu[2]; Rosa Barabash[3]; Jesper Thorborg[1]; Jesper Hattel[1]; Dorte Juul Jensen[1]; [1]Technical University of Denmark; [2]Advanced Photon Source, Argonne National Laboratory; [3]Oak Ridge National Laboratory

Ductile cast iron (DCI) has good combination of strength, ductility and fracture toughness, thanks to its composite microstructure, consisting of spherical graphite nodules (GNs) embedded in steel matrix. During manufacturing, the differences in the thermal expansion coefficients between the matrix and GN lead to local thermal residual strains/ stresses. To optimize the design and processing of DCI components, more knowledge about the magnitude of the local residual strains/ stresses is required. In this work, synchrotron X-ray microdiffraction is used to characterize microstructure and local residual strains around several GNs with different sizes in two ferritic DCIs manufactured using a permanent and sand molds. The results show that the local residual strains are mainly compressive, exhibiting gradients with maxima of 6.0-9.9×10^-4 near the GNs and decreasing into the matrix. The results are compared with those predicted from finite element modeling and discussed in relation to the GN size and cooling rate.

P-50: Methods of Visualization of Defects of Aluminum and Copper Wires: *Beata Smyrak*[1]; [1]AGH University of Science & Technology

The detection of internal material defects is one of the most important problems of modern industry. The choice of detection method depends on the shape and geometry of the product, type of material, type of defects, orientation and location of defects (internal defects, surface defects, subsurface), size of defects (eg minimum detected, minimum acceptable). The research system must be adapted to the shape of the element, its dimensions and the research issues. The paper presents the characteristics of the deffects created during the process of drawing aluminum wires and copper wires in industrial conditions. The studies of drawing deffects have been carried out using scanning microscopy and computer tomography. Based on the results of the studies, among others, the identified deffects have been classified and reasons for their occurrence have been determined.

P-51: Micro-diffraction in 3D: *Jon Tischler*[1]; [1]Argonne National Laboratory

3D Mirco-diffraction employing both white and monochromatic x-rays at the Advanced Photon Source (APS) has been a valuable capability for the last 15 years. This talk will cover the current state of 3D micro-diffraction at the APS beam line 34-ID-E. It will also describe current activities studying the diffraction from materials with spatial resolutions under 400 nm. With the planned APS upgrade, the x-ray emittance should improve by a factor of 100, providing both higher intensities and smaller resolution, with a resolution goal of 100 nm. I will also discuss other enhancements that can improve both the speed and efficiency of data acquisition. This research used the Advanced Photon Source 34-ID, a US DoE Office of Science Facility operated by Argonne National Laboratory under Contract DE-AC02-06CH11357.

P-52: Micromechanical Evolution of Ti-7Al Under Cyclic Loading: *Rachel Lim*[1]; Darren Pagan[2]; Yufeng Shen[1]; Joel Bernier[3]; Robert Suter[1]; Anthony Rollett[1]; [1]Carnegie Mellon University; [2]Cornell High Energy Synchrotron Source; [3]Lawrence Livermore National Laboratory

High-energy x-ray diffraction microscopy (HEDM), an in situ, non-destructive, 3D characterization technique, was used to track microstructural evolution in a sample of \945-phase Ti-7Al under cyclic tensile loading over the first 200 cycles. Near-field HEDM measures orientation on a regular grid which provides grain morphology, while far-field HEDM measures the strain state of each individual grain. Combined with digital image correlation (DIC), we perform grain-by-grain analysis to track strain evolution. The results show a decrease in residual elastic strain over the first cycle followed by an increasing build-up of strain. There is a broadening in the von Mises stress distribution across increasing cycles and the development of a long tail on the upper end of the distribution. Initially, the hydrostatic stress increases linearly with increasing stress coaxiality angle, and by around cycle 60-70, the trend rotates to decreasing.

P-53: Microscale Mechanisms of Tensile Deformation in Ductile Cast Iron Studied with FE Modelling and Digital Volume Correlation: *Tito Andriollo*[1]; Yubin Zhang[1]; Mathias Bjerre[1]; Søren Fæster[1]; Jesper Thorborg[1]; Jesper Hattel[1]; [1]Technical University of Denmark

The mechanisms controlling the deformation of ductile cast irons at the micro-scale are not fully clear yet. The main reason is the complex material microstructure, which consists of graphite particles embedded in a steel matrix. The present work is the first attempt to combine FE modelling and digital volume correlation to analyze how these microstructural elements interact mechanically to determine the tensile properties at the macro-scale. First, a FE model based on a representative volume element obtained from micro computed tomography (µCT) is developed and used to simulate manufacture and tensile loading of ductile cast iron. Then, the model predictions are validated via digital volume correlation, based on µCT scans acquired in-situ during deformation. The results are used to shed light on the role of the micro-scale residual stresses – associated with the thermal contraction mismatch between the graphite and the matrix during manufacture – revealed recently by the authors.

P-54: Microstructural Evolution of a ScYSZ Electrolyte of a Solid Oxide Cell at High Polarization: *José Xavier Trujillo*[1]; Jacob Bowen[1]; Henning Poulsen[1]; Peter Jørgensen[1]; Carsten Detlefs[2]; Phil Cook[2]; Hugh Simons[1]; Sonja Ahl[1]; Anders Jakobsen[1]; [1]Technical University of Denmark; [2]ESRF

Solid oxide cells are promising systems in the field of energy production and storage. When operating in harsh working conditions in electrolysis mode they exhibit degradation processes such as electrolyte grain boundary void formation, resulting in a decrease of efficiency. In this work the microstructural evolution of the electrolyte, near the anode (simulating the electrolysis oxygen evolution electrode) is assessed in-operando in a symmetrical cell composed by scandia dopped yttria stabilized zirconia (ScYSZ) and lanthanum strontium manganate / YSZ as electrolyte and electrodes respectively at 700°C in air at a polarization of 2V. A compression of lattice parameter is observed close to the anode/

electrolyte interface after 17 hours at operating conditions, attributable to oxygen pressure build up in grain boundary voids observed by post-mortem electron microscopy. Strain mapping performed by dark field X-ray microscopy revealed changes in strain domains on what we suspect are the initial stages of void formation.

P-55: Microstructure Characterization and Mechanical Analysis of Electron Beam Manufactured Ti6Al4V for Biomedical Application: *Chen Di*[1]; [1]Shanghai Jiao Tong University

Ti6Al4V has been widely used in medical treatment because of its good mechanical properties and biocompatibility. Additive manufacture, especially electron beam melting(EBM), has increasingly shown great potential for expanding the application of orthopedic implants in recent years for it can fabricate the parts individually, fast and costly. There are many studies on mechanical properties and microstructure of EBM-build parts while few of them notice that the difference in phase transformation and mechanical properties difference between thin wall or open cellar foam and bulk samples as well as. The a' transformation takes place in the laminar samples with a higher cooling rate than that of bulk samples so that the hardness of block samples is about 348.87 ±15.51HVwhile the hardness of laminar samples is about 391.55 ±12.29HV which is 12% higher than that of block samples.

P-56: Microstructure Evolution with Convection: A 3-D Phase-field-lattice Boltzmann Study Coupled with the Parallel Adaptive-mesh-refinement Algorithm: Zhipeng Guo[1]; Ang Zhang[1]; *Shaoxing Meng*[1]; Jinglian Du[1]; Shoumei Xiong[1]; [1]Tsinghua University

A high performance numerical algorithm was developed to solve the 3-D phase-filed-lattice Boltzmann equations by combining adaptive mesh refinement and parallel computing. Results showed that this approach could improve the computational efficiency by 3 orders of magnitude without compromising any accuracy. The fluid flow was induced by the imposed external force including both gravity and/or a lateral force. Influenced by the fluid flow, both dendritic and eutectic microstructures presented altered morphologies due to the convection of the solute. The fluid flow could accelerate dendritic coarsening or promote freckle formation under different configurations of the external force. Both coarsening acceleration and freckle formation could induce significant dendritic fragmentation, which agreed well with these found in synchrotron X-ray radiography experiment for the Al-Cu alloy.

P-57: Multi-Scale 3D Digital Volume Correlation of 2D material Aerogel under Compression: *Shelley Rawson*[1]; Vildan Bayram[1]; Samuel McDonald[1]; Suelen Barg[1]; Philip Withers[1]; [1]The University of Manchester

Freeze cast aerogels are highly porous structures exhibiting thin, highly aligned sheets of material, arranged in distinct domains in which the sheets lie in different planes, with struts spanning between neighbouring sheets. These aerogels are being investigated for various applications including filters, directional insulation, energy storage and biomaterials. The aerogel can also be used as a scaffold for advanced composites by infiltration with a second phase. At present, little data exists on the relationship between structural architecture and mechanical properties of these materials. We present 3D digital volume correlation via X-ray Micro-CT time lapse imaging of a 2D material aerogel during *in situ* compressive loading. Correlative imaging at multiple scales demonstrates interaction between neighbouring sheets and struts at high resolution, and how this relates more globally to interaction between different domains. These data demonstrate the relationship between features on different length-scales and the resultant mechanical properties of the bulk material.

P-58: Non-linear Iterative Methods for Direct 3D Phase-retrieval and Tomographic Inversion of Coherent Diffraction Patterns: *Tiago Ramos*[1]; Martin Andersen[1]; Jens Andreasen[1]; [1]Technical University of Denmark

Coherent X-ray diffractive imaging methods provide quantitative measurements of the sample complex refractive index with spatial resolutions on the order of tens of nanometres, high degree of penetration and minimal sample preparation when compared, for example, with electron microscopy techniques.Data processing and tomographic reconstruction from coherent diffraction data is often performed in three steps: phase-retrieval, tomographic alignment and tomographic reconstruction. We present a combined three-dimensional non-linear numerical algorithm for a direct inversion and tomographic reconstruction of far-field coherent diffraction patterns. The implementation of our algorithm allows a full flexible description of the experimental setup, generalizing its application to full-field (holography/CDI) or to scanning (ptychography) geometries, where all geometrical degrees of freedom can be defined by the user. We demonstrate the behaviour, convergence and results of our algorithm applied to simulated data, and identify the advantages of this novel reconstruction method in terms of data acquisition and data analysis.

P-59: Rapid, Easy-to-use and Powerful Segmentation by Machine Learning: *Tobias Volkenandt*[1]; Stefanie Freitag[1]; Michael Rauscher[1]; [1]Carl Zeiss Microscopy GmbH

For materials characterization it is not sufficient to just acquire images. Whenever further analysis is intended to obtain quantitative information from the sample, segmentation becomes the important task. However, although it is a crucial step in the evaluation process, researchers still tend to do it manually. This leads to less reproducible data and longer time-to-result. Additionally it often relies on threshold-based approaches, which are limited in their range of application. To solve this problem we present a new segmentation module that enables not only image analysis experts but users of any skill-level to analyze their images and benefit from machine learning. The module is available for the ZEISS ZEN software and works on any kind of image data in 2D and 3D, may it stem from light, electron or x-ray microscopy. We will illustrate its power and ease of use on several materials science datasets.

P-60: Real Time Imaging of Microstructural Transformations in Bulk Ferroelectrics: *Jeppe Ormstrup*[1]; [1]Technical University of Denmark

Ferroelectrics are a broad class of functional materials with the ability to store electric charge, convert between electrical and mechanical work, and store digital memory states. Their functionality derives from the formation and dynamics of structural domains (i.e. twins), which nucleate, reorganize and annihilate under applied electric, thermal or mechanical loads. Characterizing these processes remains a persistent challenge due to the wide range of length (nm to mm) and time (µm to minutes) scales over which they occur. Here we present the use of Dark-Field X-ray Microscopy for directly imaging and tracking individual domains in real time during phase transformations and external perturbations. We describe the methodology and its application to study electric-field induced phase transitions in barium titanate. This capability to quantitatively correlate the structural dynamics to external boundary conditions is a key requirement for formulating and validating multi-scale models that account for the full heterogeneity of ferroelectric materials.

P-61: Scanning 3DXRD Technique with a Conical Slit: *Yujiro Hayashi*[1]; Tomoyuki Yoshida[1]; Daigo Setoyama[1]; [1]Toyota Central R&D Labs., Inc.

Scanning three-dimensional x-ray diffraction (3DXRD) microscopy is a non-destructive method of 3D orientation mapping in polycrystalline materials. One of the main problems of 3DXRD-based methods is diffraction spot overlap caused by plastic deformation. We have applied a conical slit to the scanning 3DXRD method to reduce the overlap by cutting diffractions from grains outside the gauge volume formed by the slit. Orientations are mapped in the gauge volume using a focused x-ray microbeam. The scanning 3DXRD technique with a conical slit has been tested for 10%-deformed low-carbon steel sheet samples with a grain size of 20µm and a cross sectional area of $1{\times}1mm^2$. Orientations in such a highly deformed sample with a large number of grains in a cross section have been difficult to be reconstructed by 3DXRD-based methods. In our experiment, a 3D orientation map was successfully obtained using a conical slit forming a 300-µm-long gauge volume.

P-62: Stress-induced Damage Evolution in Two and Three Phase Al Matrix Composites: *Sergei Evsevleev*[1]; Sandra Cabeza[2]; Tatiana Mishurova[1]; Gerardo Garcés[3]; Guillermo Requena[4]; Igor Sevostianov[5]; Giovanni Bruno[1]; [1]Bundesanstalt für Materialforschung und -prüfung; [2]Institut Laue-Langevin; [3]National Center for Metallurgical Research CENIM; [4]German Aerospace Centre ; [5]New Mexico State University

Two metal matrix composites, both consisting of a near-eutectic cast AlSi12CuMgNi alloy, one reinforced with 15%vol. Al2O3 short fibers and the other with 7%vol. Al2O3 short fibers + 15%vol. SiC particles were studied. Distribution, orientation, and volume fraction of the different phases was determined by means of synchrotron computed tomography. The load partitioning between phases was investigated by in-situ neutron diffraction compression tests. The internal damage of the eutectic Si phase and Al2O3 fibers after ex-situ compression tests was directly observed in CT reconstructed volumes. Significant debonding between Al-matrix and SiC particles was found. Those observations allowed rationalizing the load transfer among the constituent phases of two different composites. Finally, based on the Maxwell scheme, a micro-mechanical model was utilized for the composite with one and two ceramic reinforcements. The model rationalizes the experimental data, and predicts the evolution of principal stresses in each phase.

P-63: The 3D Structure and Evolution of Porosity from Additive Manufacturing: *Richard Fonda*[1]; Jerry Feng[1]; Lily Nguyen[2]; David Rowenhorst[1]; [1]Naval Research Laboratory; [2]NRC / Naval Research Laboratory

This presentation will discuss 2D and 3D characteristics of the porosity generated during additive manufacturing of 316L stainless steel. Optical and electron microscopy, x-ray microtomography, and 3D reconstruction of serial sectioning data were used to characterize the pore morphologies, pore distributions, and the grain structure of the surrounding material in the as-built material, and reveal how these characteristics evolve during thermal and HIP post-processing.

P-64: Three-dimensional Analysis for Distribution Change of Platelet Al_3Ti Particles in Al-Al_3Ti Composite Deformed by Asymmetric Rolling Process: *Hisashi Sato*[1]; Akihiro Mori[1]; Mariko Kitagawa[1]; Sarath Babu Duraisamy[1]; Tadachika Chiba[1]; Yoshimi Watanabe[1]; [1]Nagoya Institute Of Technology

Asymmetric rolling can introduce larger shear strain than symmetric rolling. Because of this, it is expected that the asymmetric rolling for metal-based composite containing platelet particles makes different particle distribution from the symmetric rolling. Especially, size, shape and orientation of the fragmented particles in the cold-rolled composite would be much different between the asymmetric rolling and the symmetric rolling. In this study, distribution change of platelet Al_3Ti particles in Al-Al_3Ti composite by the asymmetric rolling or the symmetric rolling is investigated using 3-dimensional visualization of Al_3Ti particle. The size of the platelet Al_3Ti particles in the asymmetric rolled Al-Al_3Ti composite is smaller than that in the composite deformed by the symmetric rolling. The shape of the Al_3Ti particles in the composites deformed by both rolling processes remains platelet shape. Also, it is found that the Al_3Ti particles are preferentially fragmented along $\{112\}_{Al3Ti}$.

P-65: Through-process Quantification of Additive Manufactured Industrial Parts Using X-ray Micro-tomography: *Sheng Yue*[1]; Peter Lee[2]; Chunlei Qiu[3]; Aymeric Beau[1]; Moataz Attallah[3]; Philip Withers[2]; [1]North Star Imaging, UK; [2]University of Manchester; [3]University of Birmingham

Powder bed additive manufacturing (AM) technologies have been growingly used to fabricate real life industrial parts. However, one remaining and critical challenge is to validate and qualify these parts for their intended functionalities in a cost and time efficient way. High resolution industrial X-ray microtomography has proven to be a powerful non-destructive tool to aid the design, process optimisation, quality control, and quality assurance in AM.Here, we first demonstrated how to optimise scanning modes and parameters to meet the time and resolution requirement for production. Using our bespoke program, more than 60,000 gas atomised metallic powders were scanned and quantified for the size and shape distribution, inclusion percentage, etc. For as-fabricated and final processed parts, key quality indicators, such as morphology descriptors, defects level and distribution, and 3D surface finishing quality and distribution were accurately and robustly obtained. Finally, an X-ray CT based through-process quality monitoring frame was proposed.

P-66: Use of Disposable Rulers for Measuring Slice Thickness during FIB Tomography: *Helen Jones*[1]; Ken Mingard[1]; David Cox[1]; [1]National Physical Laboratory

3D microstructural reconstructions from focussed ion beam milling usually assume uniform slice thicknesses. Measurements on artificial structures with known dimensions have shown that this is not the case. Fiducial markers can be used but require deposition and marking of features of known geometry but this can be time consuming and difficult to produce accurately each time. A process has been developed to “mass produce“ rulers on 100 nm silicon nitride films which can be quickly cut in the FIB and lifted into position with a micromanipulator. This paper will describe the development of the optimum geometry for the rulers using FIB deposition of multiple markers at 45degrees to the milled face and then discuss how this information has been applied with a lithography process to produce multiple rulers. Examples will be shown of the lift out and positioning of the pre-formed rulers for use with real life microstructures.

P-67: Visualisation and Measurement of Hardmetal Microstructures in 3D: Ken Mingard[1]; Bryan Roebuck[1]; *Helen Jones*[1]; Mark Stewart[1]; David Cox[1]; Mark Gee[1]; [1]National Physical Laboratory

Two phase Hardmetal microstructures have been well characterised in 2D and relationships, often only empirical, have been derived which relate key properties such as wear resistance to e.g. WC grain size. The question remains how representative the 2D relationships are of the true 3D structure and whether a 3D view would enable better visualisation and modelling of hardmetals’ properties.EBSD and FIB has been used to produce 3D reconstructions of several hardmetal grades and 2D and 3D grain size distributions of WC compared. A close correspondence between the two is observed if the smallest grain size fractions are excluded. Aspect ratios vary widely with size but false impressions of more needle like grains can be produced by neighbouring multiple particles of almost identical orientation. New insights into the continuous Co binder phase network have been obtained while the 3D shapes of WC grains can be related to their crystallographic orientation.

P-68: 3D Investigation on Colloidal Crystals by Synchrotron Radiation Phase-contrast Computed Tomography: *Yanan Fu*[1]; [1]Shanghai Institute of Applied Physics, Chinese Academy of Sciences

The three dimensional (3D) void system of the colloidal crystal was noninvasively characterized by synchrotron radiation phase-contrast computed tomography, and the quantitative image analysis was implemented. Comparing with gravity sedimentation method, the samples fabricated from floatage self-assembly with mixed solvents have the lowest porosity, and when ethylene glycol and water were mixed with ratio of 1:1, the lowest porosity of 27.49% could be achieved. In single slices, the porosities and fractal dimension for the voids were calculated. The results showed that two factors would significantly influence the porosity of the whole colloidal crystal: the first deposited sphere layer’s orderliness and the sedimentation speed of the spheres. The floatage self-assembly could induce a stable close-packing process, resulted from the powerful nucleation force-lateral capillary force coupled with the mixed solvent to regulate the floating upward speed for purpose of matching the assembly rate.

P-69: In-situ 3D Measurement of Surface Relief Induced by Phase Transformation in Low Carbon Steel by Digital Holographic Microscope: *Shuehi Komine*[1]; Junya Inoue[1]; [1]The University of Tokyo

Digital holographic microscope (DHM) was applied to in-situ measure surface relief (SR) accompanied by the formation of plate-like microstructures in low carbon steels. SR was conventionally measured by scanning microscopes at room temperature in order to investigate the mechanism of phase transformations. DHM can measure the change of 3D shape of the surface even when the formed structures are being surrounded by austenite because of its non-contact method and high measurement rate as over 50 fps. Therefore, more rigorous investigations are possible into the mechanism. The pure deformation by the transformation can be acquired by subtracting the height of the surface just before the transformation from the height of the deformed surface. We verified the applicability of phenomenological theory of martensite crystallography (PTMC) for the shape of SR by comparing the measured shape with the estimated shape by PTMC in combination with a crystal orientation analysis.

P-70: A New Generation of X-ray Computed Tomography Devices for Quality Assurance and Metrology Inspection in the Field of Additive Manufacturing: *Andre Beerlink*[1]; [1]YXLON International GmbH

The YXLON FF35 CT system is designed to achieve extremely precise X-ray inspection results for a wide range of applications while at the same time it offers user friendliness at highest level by a new intuitive touch interface control concept and further smart functionalities. With its metrology capabilities it is perfect for very small to medium size parts inspection in the quality assurance for automotive, electronics, aerospace and material science industries and research. Results of representative applications, e.g. from additive manufacturing, metrology and carbon fibre composites, will be highlighted during the presentation to demonstrate the performance of today´s laboratory CT devices, such as the YXLON FF35 CT, and how they are used to increase the level of quality assurance processes in 3D materials sciences.

P-71: Lab Based Diffraction Contrast Tomography – Applications and Future Directions: *James Carr*[1]; Samuel McDonald[1]; Hrishikesh Bale[2]; Nicolas Gueninchault[3]; Erik Lauridsen[3]; Philip Withers[1]; [1]University of Manchester; [2]Carl Zeiss Microscopy Inc.; [3]Xnovo Technology ApS

The mechanical properties of polycrystalline materials are significantly affected by behaviour at the crystalline grain structure level. The ability to characterise crystallographic microstructure in 3D, or 3D through time, non-destructively, is a powerful tool for understanding materials performance. The recent diffraction contrast based X-ray tomography technique (LabDCT) allows routine characterization of polycrystalline materials on a commercial laboratory X-ray microscope. Combining grain orientation and microstructural information opens new possibilities for characterization of damage, deformation and growth mechanisms. Imaging these microscopic features in 3D with advanced contrast techniques enhances the collective understanding of fundamental materials mechanisms behind these processes. Here, we present select application examples of LabDCT, including the following of grain growth and grain reorientation during sintering of copper, influence of crystallography on corrosion in Mg alloys and identification of large grains in nickel-base superalloys. Results compared against serial section SEM-EBSD measurements will also be discussed.

P-72: Large-scale Phase-field Simulation of 3D Ideal Grain Growth: Testing the Mean-field Theory and Stereological Analysis: *Eisuke Miyoshi*[1]; Tomohiro Takaki[1]; Munekazu Ohno[2]; Yasushi Shibuta[3]; Shinji Sakane[1]; Takashi Shimokawabe[3]; Takayuki Aoki[4]; [1]Kyoto Institute of Technology; [2]Hokkaido University; [3]The University of Tokyo; [4]Tokyo Institute of Technology

Grain growth is one of the most fundamental phenomena in controlling the microstructure of polycrystalline materials. However, the true picture of grain growth is still controversial even for the simplest (or ideal) case, mainly due to the difficulty in extracting reliable statistics for 3D grain assemblies from experiments or limited-scale simulations. In this study, by utilizing the phase-field method and parallel GPU computing on a supercomputer, we perform ultra-large-scale simulations of 3D ideal grain growth with up to 2560^3 grids and more than three million initial grains. This computational scale allows for quantifying the grain growth behaviors with a quite-high degree of statistical reliability. On the basis of the simulated results and mean-field theory, a predictive model of ideal grain growth is discussed. Furthermore, the applicability of the stereological analysis to ideal growth is tested, demonstrating that the 3D microstructural characteristics in this phenomenon can be inferred from cross-sectional observations.

P-74: Permeability Prediction for 3D Dendrites Structure by Large-scale Phase-field Lattice Boltzmann Simulation: *Tomohiro Takaki*[1]; Shinji Sakane[1]; Munekazu Ohno[2]; Yasushi Shibuta[3]; Takayuki Aoki[4]; [1]Kyoto Institute of Technology; [2]Hokkaido University; [3]The University of Tokyo; [4]Tokyo Institute of Technology

To perform a macroscopic casting simulation with high accuracy, we need permeability data for the interdendritic liquid flow. There are experimental and numerical ways to acquire the permeability data. The experimental way to obtain the permeability have been mainly studies in the 1990s. In the experimental method, a systematical permeability prediction for various dendrite structures is difficult. Therefore, a permeability prediction by numerical simulation is expected as a promising way. Here, a problem in the numerical way is a high computational cost. In this study, we enable a systematical permeability prediction for three-dimensional (3D) complicated dendrite structure by GPU-accelerated large-scale simulation. In this method, we use a phase-field method for the dendrite structure prediction, and lattice Boltzmann method for the prediction of interdendritic liquid flow. The simulation is accelerated by a GPU supercomputer TSUBAME3.0 at Tokyo Institute of Technology. Some simulation examples are introduced in this presentation.

P-73: Advanced 3D Classification of Graphite in Cast Iron: *Andres Olguin*[1]; Michael Engstler[1]; Emilio Jimenez Piqué[2]; Frank Mücklich[1]; [1]Saarland University; [2]Universitat Politècnica de Catalunya

Visual analysis classification of graphite in cast iron is an established method in the foundry industry. It is the metallographer's task to estimate the percentages of the different graphite forms and sizes. The European Standard EN ISO 945-1 defines 6 graphite forms: I (lamellar), II (crab), III (vermicular), IV (temper carbon), V (slightly irregular spheroidal) and VI (spheroidal); and provides reference micrographs for comparison. A natural shortcoming of this method is its inherent subjectivity. In this project, we seek to develop a routine for objective classification based on 3D data obtained from serial polishing and micro-computed tomography. Planar sections of reconstructed volume elements are used to estimate probability distributions of parameters proved relevant in graphite characterisation. The practical application of these probability distributions is as calibration (i.e. decision) curves in a classifier.

P-75: Finite-deformation Continuum Dislocation Dynamics for 3D Dislocation Microstructure: *Anter El-Azab*[1]; [1]Purdue University

Most dislocation dynamics model developments focus on the simulation of line dynamics and density based, statistical mechanical approaches for dislocation evolution for the case of infinitesimal crystal deformation. We present a finite deformation, density based dislocation dynamics approach for mesoscale deformation of single crystals. This framework is a generalization to finite deformation of our earlier successful model for dislocation microstructure evolution based on continuum dislocation dynamics. A derivation of the dislocation transport equations at finite strain and lattice rotation in Lagrangian and Eulerian forms is outlined, with a special focus on the kinematic coupling of dislocation density evolution on individual slip systems and to the coupling via cross slip and dislocation reactions. The relevant crystal mechanics, thermodynamics, and constitutive closure questions will be discussed.

P-76: High Resolution X-ray Microscopy and 3D Simulations for Ceramics: *Alisa Stratulat*[1]; [1]Carl Zeiss Microscopy Limited

The development of new advanced ceramics for industrial applications (insulators, membranes for separation and filtration, etc.) relies on the understanding of the material structure and process optimization. Traditional characterization methods for these materials often imply complicated and time-consuming sample preparation and only analyse small volumes within the sample. Hence, there is a need for more advanced techniques that provide better understanding of the performance of these materials. 3D X-Ray Microscopy (XRM) provides methods for imaging and analysis of ceramics such as porosity measurement throughout the volume of interest, identification and segmentation of different phases and non-destructive observations of internal defects or voids. In addition, real 3D structures are generated that can be imported into simulation models to predict effective diffusivity, fluid flow or thermal properties. This presentation will overview the advantages of coupling XRM with physics simulations and illustrate some applications in the area of ceramics.

P-77: In-situ Characterization of Subgrains by 3D High Resolution Reciprocal Space Mapping during Cyclic Deformation: *Annika Diederichs*[1]; Ulrich Lienert[2]; Henning Friis Poulsen[1]; Wolfgang Pantleon[1]; [1]Technical University of Denmark; [2]DESY Photon Science, Deutsches Elektronen Synchrotron

High Resolution Reciprocal Space Mapping uses a focused beam of high energy X-rays to provide quantitative information about the internal structure of individual grains embedded in a macroscopic sample by acquiring three-dimensional intensity distributions with high angular resolution. Because of local differences in the crystalline lattice of deformed metals, the collected reciprocal space maps do not show a smooth intensity distribution. Dislocation-free subgrains can be identified by distinct intensity peaks, while dislocation-rich walls manifest as a smooth cloud with lower intensity. The substructure within individual grains can thus be analyzed and internal stresses revealed. The evolution of a large number of subgrains can be followed in-situ during loading sequences, which is demonstrated on polycrystalline aluminium during tension-compression cycling. The radial peak positions of the individual subgrains follow a Gaussian distribution indicating variations in their specific elastic strains; these develop with proceeding deformation in overall accordance with refined composite models.

P-78: Innovative Imaging Developments at the PSICHE Beamline of Synchrotron SOLEIL: *Andrew King*[1]; Nicolas Guignot[1]; Jean-Pierre Deslandes[1]; Eglantine Boulard[2]; Yann Le Godec[2]; Jean-Paul Itié[1]; [1]Synchrotron SOLEIL; [2]IMPMC, UMPC

The PSICHE beamline of the SOLEIL synchrotron performs tomography and diffraction experiments, primarily for materials science and geophysics users. Here we describe a series of recent innovations that extend the capabilities of the instruments, and present examples of results obtained. Stepwise, high vertical overlap tomography allows ring artefacts to be substantially reduced at the acquisition stage, especially important in samples presenting low contrast or in which rings are difficult to correct post acquisition. Scanning radiography with a line focused beam allows 2D imaging to be combined with efficient diffraction measurements. The UToPEC project is a new Paris-Edinburgh press optimised for high speed tomography (0.5 seconds per full tomogram) at high pressures and temperatures (up to 10GPa and 1500K).

P-79: Mesoscopic Simulations of Pristine and Cross-linked Carbon Nanotube Films: Structural and Mechanical Properties: *Alexey Volkov*[1]; Abu Horaira Banna[1]; [1]University of Alabama

Relationships between structural and mechanical properties of carbon nanotube (CNT) films are studied numerically based on a mesoscopic model of CNT materials. In the mesoscopic model, every nanotube is represented as a chain of stretchable cylindrical segments. The mesoscopic force field accounts for stretching, bending, and bending buckling of CNTs as well as for van der Waals intertube interaction and presence of covalent cross-links. The CNT films are generated in dynamic simulations of self-organization of initially dispersed CNTs into a stable continuous network of bundles. The structural parameters of the generated films are compared with the properties obtained in experimental studies. The elastic and inelastic properties of generated CNT films are found in simulations of stretching and compression under conditions of quasi-static and dynamic loading. The calculated elastic moduli and material strength are correlated with the CNT length, material density, cross-link density, and structural parameters of CNT networks.

P-80: Multi-scale Analysis of Deformation in Ductile Cast Iron Using Combined 3DXRD, X-ray Tomography, Image Analysis and Digital Volume Correlation: *Stephen Hall*[1]; Torsten Sjögren[2]; Erik Dartfeldt[2]; Peter Skoglund[3]; Lennart Elmquist[4]; Marta Majkut[5]; Jonas Engqvist[1]; Jessica Elfsberg[3]; [1]Division of Solid Mechnics, Lund University; [2]Research Institutes of Sweden; [3]Scania; [4]SWEREA; [5]European Synchrotron Radiation Facility

Ductile cast irons (DCI) are often the preferred materials, e.g., for the exhaust systems of heavy truck engines, due to their greater ductility and, thus, greater strength and fatigue resistance, compared to other cast irons. DCI comprises a ferrite matrix with dispersed graphite spheroids, which impedes crack development. The mechanical response of DCI is, thus, a complex, multi-scale interaction of different material phases. Here, deformation in DCI is studied over different length-scales during in-situ tensile testing at beamline ID11, ESRF. We focus on the use of in-situ 3DXRD to study the evolution of the strain in the crystalline ferrite matrix and correlate this with continuum strain fields from digital volume correlation of x-ray tomography images acquired at the same load levels. Furthermore, deformation in the graphite nodules is assessed by image analysis. In combination, the results provide new insights into the multi-scale coupling of deformation in DCI.

P-86: Initial Efforts Towards Molecular Dynamics Modelling of Mesoscale Bulk Heterojunction Morphologies: *Anders Gertsen*[1]; Drew Pearce[2]; Anne Guilbert[2]; Jenny Nelson[2]; Jens Andreasen[1]; [1]Technical University of Denmark; [2]Imperial College London

Organic photovoltaics based on polymer:fullerene or polymer:polymer active layers are crucially dependent on the three-dimensional (3D) morphology of the mesoscale bulk heterojunction due to the limited exciton diffusion lengths in polymeric materials. Here, we present Molecular Dynamics (MD) simulations of single indacenodithiophene-co-benzothiadiazole (IDTBT) polymers in solution and the dependence of their properties such as persistence lengths on different sidechains and solvents, since long persistence lengths are believed to be crucial for high charge mobilities. Furthermore, we present initial efforts towards reaching mesoscale simulations by employing coarse-grained MD models, i.e. decreasing the number of degrees of freedom through the description of several atoms in a unified manner, in the search of obtaining time-resolved insight into the bulk heterojunction formation. Through this, we hope to aid the interpretation of experimental 3D imaging and refine the current, predominantly phenomenological, hypotheses which are based on indirect experimental probing of 3D morphology.

P-81: Observing Thermal-driven Martensitic Phase Transformation in NiTi Single Crystals Below the Surface and in High Resolution: *Ashley Bucsek*[1]; Jeppe Ormstrup[2]; Mustafacan Kustal[3]; Can Yildirim[3]; Phil Cook[3]; Hugh Simons[2]; Carsten Detlefs[3]; Aaron Stebner[1]; [1]Colorado School of Mines; [2]Technical University of Denmark; [3]European Synchrotron Radiation Facility

The promise of shape memory alloys (SMAs) has led to over 20,000 patents worldwide. However, the promise of SMAs has not been matched by its technological impact—only a limited number of these patents have been realized as commercially viable. One reason for this gap between development and implementation is the lack of suitable experiments. The length scales of microstructure interfaces in an SMA routinely span 10 nm to 1 mm, and techniques which can be used at these length scales are typically limited to surface observations, are destructive, or are averaged over many grains. Dark-Field X-Ray Microscopy (DFXM) offers the capability to measure through bulk specimens with a spatial resolution of 100 nm, and orientation and strain sensitivities of 0.1 mrad and 10-4, respectively. We present the first-ever DFXM experiments on SMAs, which include in-situ, below-the-surface observations of thermal-driven martensitic phase transformation in single-crystal NiTi SMAs.

P-82: OOF 3D: New Developments in a Materials-focused Finite Element System: *Andrew Reid*[1]; [1]National Institute of Standards and Technology

The OOF object-oriented finite element software provides a finite-element tool with a GUI interface designed around the needs and knowledge of materials science domain experts, packaging sophisticated image-processing and finite element algorithms in a way that encourages structure-property exploration. A major feature of this code is a suite of tools to allow users to construct well-formed, space-filling 3D meshes with boundaries that match up with features in the input microstructure image. This presents an interface design and visualization challenge in 3D in particular, where generalization from 2D has not been straightforward. In particular, the development team has recently incorporated a new algorithm for computing the homogeneity of candidate finite elements, an important aspect of numerically assessing mesh quality, which can be difficult to assess visually in 3D. This talk will review the current state of both the user-interface and technical capabilities of OOF 3D.

P-83: Phase Field Modeling of Grain Boundary Evolution in Porous Oxides: *Anter El-Azab*[1]; [1]Purdue University

We present a phase field model for investigating grain boundary evolution in porous oxides with applications to UO2 and CeO2. The model takes into account the interactions between pores and grain boundaries as well as the pore mobility effects. Using a formal asymptotic analysis, the phase field model was matched to its sharp-interface counterpart and all model parameters were uniquely determined. Therefore, the model is able to obtain accurate growth rates that can be compared with experiments. The model was used to reveal various growth regimes in porous oxides and sort the boundary-controlled versus pore-controlled growth kinetic regimes. The model results showed that the pore breakaway phenomenon can only be observed in 3D simulations. The important features of the model and results will be presented.

P-84: Pseudo-3D Modelling of Sigma Phase Precipitation in a Duplex Stainless Steel: *Anders Salwén*[1]; [1]InnoXinetix AB

Computer modelling of sigma phase nucleation, growth and dissolution in a duplex stainless steel will be compared to measurements ("In-Situ Observations of Sigma Phase Dissolution in 2205 Duplex Stainless Steel using Synchrotron X-Ray Diffraction", J.W. Elmer, T.A. Palmer and E.D. Specht, 2006). Austenite and sigma phase are modeled as spheres with a sharp interface, each phase with a discrete size distribution. Pseudo-3D denotes that the diffusion fields are 3D in the spherical precipitates (treated as point sources) and their close matrix surroundings and maximum 1D in the remaining matrix. Diffusion of Cr, Mo, Ni and N is modelled using mobilities and chemical potentials from Thermo-Calc databases. All spheres of austenite and sigmaphase interact with each other via exchange of alloying elements via the ferrite matrix. The dynamics of the system, i.e. the growth or shrinkage of the spheres, is determined by maximizing the decrease of the total Gibbs energy of the system for each time step. No assumption is made about the interface compositions, such as "local equilibrium", which, together with surface energies, makes it possible to describe Ostwald ripening.Nucleation in the ferrite is determined by equilibrium calculations and the incubation time before nucleation takes place is determined by the user.

P-85: Three-dimensional Phase-field-lattice Boltzmann Modelling of Dendritic and Eutectic Growth with Coupled Heat and Solute Diffusion: *Ang Zhang*[1]; Jinglian Du[1]; Shaoxing Meng[1]; Zhipeng Guo[1]; Shoumei Xiong[1]; [1]Tsinghua University

The interaction of thermal and solute diffusion determines the morphological evolution during solidification, which significantly influences the eventual mechanical properties of materials. The phase-filed models were further extended to simulate the pattern evolution with coupled heat and solute diffusion by applying the lattice Boltzmann method to solve temperature filed equation, which has good stability and less constraint on the time step. To improve the computational efficiency, a parallel-adaptive mesh refinement algorithm was employed to reduce the computation load and economize the memory. Full solute and thermal coupling was achieved for Al-Cu alloy with a realistic Lewis number (Le, ~ 10^4). 3-D simulations on dendritic and eutectic growth under multi-scale thermal-solute condition was first performed. Results showed that the thermal diffusivity capacity had remarkable difference on the final microstructure morphology. The increasing Le would lead to a great difference including the pattern and growth velocity.

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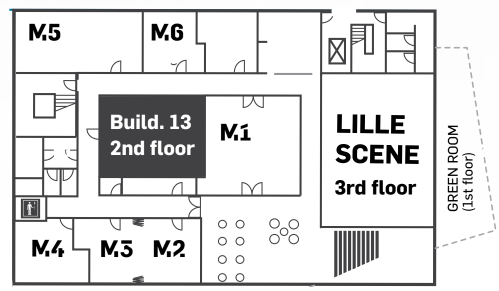
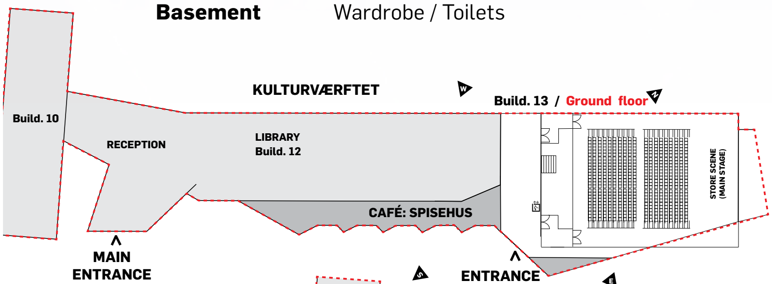
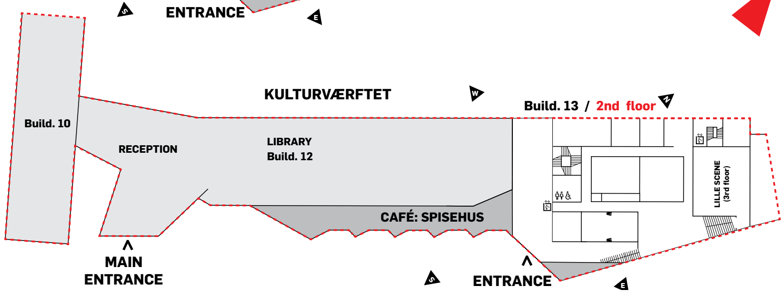
KULTURVÆRFTET (CULTURE YARD) CONFERENCE CENTER

All meeting and conference facilities are located in building 13. There is access through the main entrance in building 12 or through the entrance directly outside building 13.

4th floor	Roof Terrace
3th floor	Lille Scene
2nd floor	Meeting Rooms M1 - M6
1st floor	The Balcony of Store Scene, Green Room, Prismen
Ground floor	Store Scene, Café: Spisehuset
Basement	Wardrobe / Toilets







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