



Frontiers of Quantification and Predictive Capability in Physical Metallurgy

July 23 - 28, 2017

Chairs

Peter Gumbsch and Ji-Cheng Zhao

Vice Chairs

Carol A. Handwerker and Dierk R. Raabe

University of New England

11 Hills Beach Road
Biddeford, ME, US

Conference Description

The field of Physical Metallurgy is currently seeing major changes in its research aims from qualitative understanding to quantitative predictive capability. This is largely driven by our ability to handle massive 3D data describing the structure of materials, to locally evaluate materials properties, and to acquire systematic data series in high-throughput experiments. As 3D imaging is transitioning from technique development to application, it permits one to test modeling approaches at different levels of complexity and spatial resolution. Here, the direct modeling and simulation of experiments and the inverse modeling of the experimental results just begin to demonstrate their analytic power and their power to increase the accuracy of the measurements. Meanwhile, the classical core of the field, modelling of materials behavior and of structure-property relations, is still challenged by the difficulties to seamlessly transition between different modelling scopes from atoms to materials defects to continuum field equations. The frontiers of the field therefore are concerned with the systematization and the quantification of information on materials and with the assessment and increase of the predictive capability of the modelling and simulation. Modelling and simulation is beginning to provide thermodynamic information on materials in complex environments. Small scale experiments can be pushed to the scale of individual defects and can challenge modelling particularly concerning the mechanical properties of materials: fracture, fatigue, friction and wear. Additive manufacturing is posing new challenges to modelling and at the same time opens entirely new avenues to alloy development. The aim of this Gordon Conference is to assess these current frontiers of the field and to sketch central questions which the community will



have to solve for Physical Metallurgy to advance as a field that spans from understanding atomistic processes on femtosecond time scales to assessing the behavior of structural components for years in service.

Related Meeting



This GRC will be held in conjunction with the "Physical Metallurgy (GRS)" Gordon Research Seminar (GRS). Those interested in attending both meetings must submit an application for the GRS in addition to an application for the GRC. Refer to the [associated GRS program page](#) for more information.

Conference Program

| Sunday | |
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| 2:00 pm - 9:00 pm | Arrival and Check-in |
| 6:00 pm - 7:00 pm | Dinner |
| 7:30 pm - 7:40 pm | Introductory Comments by GRC Site Staff / Welcome from the GRC Chair |
| 7:40 pm - 9:30 pm | Learning Across Disciplines and Dealing with Big Data Discussion Leader: Dennis Dimiduk (Ohio State University, USA) |
| 7:40 pm - 8:20 pm | William Schroeder (Kitware Inc. , USA) "Frontiers in Image Analysis: Past, Present and Future" |
| 8:20 pm - 8:35 pm | Discussion |
| 8:35 pm - 9:15 pm | Nicholas Bassill (New York State Mesonet / University at Albany, SUNY, USA) "Numerical Weather Prediction" |
| 9:15 pm - 9:30 pm | Discussion |
| Monday | |
| 7:30 am - 8:30 am | Breakfast |



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| 9:00 am - 12:30 pm | Multi-Scale Assessment of Mechanical Properties Discussion Leader: Victoria Miller (North Carolina State University, USA) |
| 9:00 am - 9:40 am | Henry Proudhon (MINES ParisTech, France) "Using Near-Field X-Ray Imaging and Diffraction to Study the Mechanics of Polycrystalline Materials" |
| 9:40 am - 10:00 am | Discussion |
| 10:00 am - 10:30 am | Coffee Break |
| 10:30 am - 11:10 am | Jaafar El-Awady (Johns Hopkins University, USA) "Quantifying Fatigue Damage and Crack Initiation in Metals: Coarse-Grained Simulations and <i>In Situ</i> Experiments" |
| 11:10 am - 11:30 am | Discussion |
| 11:30 am - 12:10 pm | Joel Bernier (Lawrence Livermore National Laboratory, USA) " <i>In Situ</i> Characterization for Polycrystalline Materials at the Intergranular Mesoscale" |
| 12:10 pm - 12:30 pm | Discussion |
| 12:30 pm - 1:30 pm | Lunch |
| 1:30 pm - 4:00 pm | Free Time |
| 4:00 pm - 6:00 pm | Poster Session |
| 6:00 pm - 7:00 pm | Dinner |
| 7:30 pm - 9:30 pm | Interfaces in Functional Materials Discussion Leader: Guenter Gottstein (RWTH Aachen University, Germany) |
| 7:30 pm - 8:10 pm | Ju Li (Massachusetts Institute of Technology, USA) "Interfaces in Environments" |
| 8:10 pm - 8:30 pm | Discussion |
| 8:30 pm - 9:10 pm | Cynthia Volkert (University of Goettingen, Germany) "Controlling Friction at Nanoscale Sliding Contacts" |



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| 9:10 pm - 9:30 pm | Discussion |
| Tuesday | |
| 7:30 am - 8:30 am | Breakfast |
| 8:30 am - 9:00 am | Group Photo |
| 9:00 am - 12:30 pm | Frontiers in Alloy Design Discussion Leader: David Rugg (Rolls Royce, United Kingdom) |
| 9:00 am - 9:40 am | Rui Yang (Institute of Metal Research, Chinese Academy of Sciences, China) "Alloy and Process Design for High Performance Titanium Alloys and Aluminides" |
| 9:40 am - 10:00 am | Discussion |
| 10:00 am - 10:30 am | Coffee Break |
| 10:30 am - 11:10 am | Kevin Anderson (Mercury Marine, Brunswick Corporation, USA) "Metallurgy of Sustainable, High Toughness, Al-Si High Pressure Die Casting Alloys" |
| 11:10 am - 11:30 am | Discussion |
| 11:30 am - 12:10 pm | William Curtin (École Polytechnique Fédérale de Lausanne, Switzerland) "Predictive Theory to Guide Design of High Entropy Alloys" |
| 12:10 pm - 12:30 pm | Discussion |
| 12:30 pm - 1:30 pm | Lunch |
| 1:30 pm - 4:00 pm | Free Time |
| 4:00 pm - 6:00 pm | Poster Session |
| 6:00 pm - 7:00 pm | Dinner |
| 7:30 pm - 9:30 pm | Small Scale Experiments Testing the Big Discussion Leader: Kevin Hemker (Johns Hopkins University, USA) |



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| 7:30 pm - 8:10 pm | Mitra Taheri (Drexel University, USA) "Small Scale <i>In Situ</i> Experiments: Opportunities for New Science and Avoiding the Pitfall of Simply Scaling Down the Bulk" |
| 8:10 pm - 8:30 pm | Discussion |
| 8:30 pm - 9:10 pm | Daniel Gianola (University of California, Santa Barbara, USA) "Recent Advances in Quantitative <i>In Situ</i> Mechanical Testing: Towards High-Throughput Defect Analysis" |
| 9:10 pm - 9:30 pm | Discussion |
| Wednesday | |
| 7:30 am - 8:30 am | Breakfast |
| 9:00 am - 12:30 pm | Microstructure Prediction Beyond Classical Thermodynamics Discussion Leader: Dierk Raabe (Max Planck Institute for Iron Research, Germany) |
| 9:00 am - 9:40 am | Anton Van der Ven (University of California, Santa Barbara, USA) "High Temperature Thermodynamics of Alloys and Their Oxides from First Principles" |
| 9:40 am - 10:00 am | Discussion |
| 10:00 am - 10:30 am | Coffee Break |
| 10:30 am - 11:10 am | Maryam Ghazisaeidi (Ohio State University, USA) "Multi-Cell Monte Carlo Method for Phase Prediction in Alloys" |
| 11:10 am - 11:30 am | Discussion |
| 11:30 am - 12:10 pm | Marisol Koslowski (Purdue University, USA) "Stress Relaxation Mechanisms in Nano Crystalline Thin Films" |
| 12:10 pm - 12:30 pm | Discussion |
| 12:30 pm - 1:30 pm | Lunch |
| 1:30 pm - 4:00 pm | Free Time |



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| 4:00 pm - 6:00 pm | Poster Session |
| 6:00 pm - 7:00 pm | Dinner |
| 7:30 pm - 9:30 pm | 3D Microstructures Discussion Leader: Alexis Lewis (National Science Foundation, USA) |
| 7:30 pm - 8:10 pm | Yujiro Hayashi (Toyota Central R&D Labs., Inc., Japan) "3D Orientation and Stress Mapping with X-Ray Diffraction" |
| 8:10 pm - 8:30 pm | Discussion |
| 8:30 pm - 9:10 pm | Tresa Pollock (University of California, Santa Barbara, USA) "3D Microstructure: Promise, Progress and Barriers" |
| 9:10 pm - 9:30 pm | Discussion |

Thursday

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| 7:30 am - 8:30 am | Breakfast |
| 8:30 am - 9:00 am | Business Meeting <i>Nominations for the Next Vice Chair; Fill in Conference Evaluation Forms; Discuss Future Site and Scheduling Preferences; Election of the Next Vice Chair</i> |
| 9:00 am - 12:30 pm | Frontiers in Additive Manufacturing Discussion Leader: Jutta Kloewer (VDM Metals, Germany) |
| 9:00 am - 9:40 am | Moataz Attallah (University of Birmingham, United Kingdom) "Additive Manufacturing of Ni-Superalloys" |
| 9:40 am - 10:00 am | Discussion |
| 10:00 am - 10:30 am | Coffee Break |
| 10:30 am - 11:10 am | Sudarsanam Suresh Babu (University of Tennessee, USA) "Transients in Solidification and Solid-State Transformations in Materials During Additive Manufacturing with Complex Thermo-Mechanical Signatures" |
| 11:10 am - 11:30 am | Discussion |



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| 11:30 am - 12:10 pm | Michael Groeber (Air Force Research Laboratory, USA) "Application of Characterization, Modeling and Analytics Towards Understanding the Process-Structure Linkages in Metallic 3D Printing" |
| 12:10 pm - 12:30 pm | Discussion |
| 12:30 pm - 1:30 pm | Lunch |
| 1:30 pm - 4:00 pm | Free Time |
| 4:00 pm - 6:00 pm | Poster Session |
| 6:00 pm - 7:00 pm | Dinner |
| 7:30 pm - 9:30 pm | Direct Modelling of Experiments Discussion Leader: Carol Handwerker (Purdue University, USA) |
| 7:30 pm - 8:10 pm | Marc De Graef (Carnegie Mellon University, USA) "Enabling Quantitative Microstructure Analysis Through Forward Modeling of Characterization Modalities" |
| 8:10 pm - 8:30 pm | Discussion |
| 8:30 pm - 9:10 pm | Christopher Hutchinson (Monash University, Australia) "Combinatorial Approaches in Metallurgy – Transitions in Behaviour, Model Calibration and Interfacial Properties" |
| 9:10 pm - 9:30 pm | Discussion |
| Friday | |
| 7:30 am - 8:30 am | Breakfast |
| 9:00 am | Departure |

Contributors

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|  Gordon Research Conferences |  Carl Storm Underrepresented Minority Fellowship |  |
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