

SYMPOSIUM CM2

Advanced Numerical Algorithms for Metallic Systems at the
Mesoscale in Materials Science
April 18 - April 20, 2017

Symposium Organizers

Laurent Capolungo, Georgia Institute of Technology
Enrique Martinez, Los Alamos National Laboratory
Daniel Schwen, Idaho National Laboratory
Aurelien Vattre, Commissariat a l'energie atomique

Proceedings Statement

All authors are invited to submit articles based on their 2017 MRS Spring Meeting presentations to the journals in the MRS portfolio (www.mrs.org/publications-news). Papers submitted and accepted for publication in MRS Advances (www.mrs.org/mrs-advances) will be available as symposium collections. Visit the MRS/Cambridge University Press Publications Booth #100 in the Exhibit Hall to learn more, including MRS Advances print options available at special rates during the meeting week only.

* Invited Paper

SESSION CM2.1: Input to Mesoscale Modeling
Session Chair: Enrique Martinez
Tuesday Morning, April 18, 2017
PCC North, 100 Level, Room 125 B

10:45 AM *CM2.1.01
Reconciling Ab Initio Modeling of Self-Interstitial Migration with Internal Friction Experiments in Irradiated Zirconium [Emmanuel Clouet](#); CEA Saclay, France.

11:15 AM CM2.1.02
Point Defects in Materials—Measurement of Elastic Dipoles and Polarisability Effects [Celine Varvenne](#); CINaM - CNRS / Aix-Marseille University, France.

11:30 AM CM2.1.03
Coarse Grained Molecular Dynamic Simulations of the Interaction of a Carbon Nanotube with a Bilayer Membrane [Clarence Matthai](#); Cardiff University, United Kingdom.

SESSION CM2.2: Beyond Atomistic Models I
Session Chair: Emmanuel Clouet
Tuesday Afternoon, April 18, 2017
PCC North, 100 Level, Room 125 B

1:30 PM *CM2.2.01
A Coupled Continuum-Atomistic Framework for 2D Layered Heterostructures [Ellad B. Tadmor](#); University of Minnesota, United States.

2:00 PM CM2.2.02
Quantifying the Complex Dynamics of Moving Dislocations from the Atomic to the Microscale [Rigelesaiyin Ji](#); Iowa State University, United States.

2:15 PM *CM2.2.03
Static Strain Aging—A Diffusive Molecular Dynamics Study [Chad Sinclair](#); University of British Columbia, Canada.

2:45 PM BREAK

3:15 PM CM2.2.04
First-Principles and Grand Canonical Monte Carlo Simulations of Pseudocapacitive Response of MnO₂ Electrodes [Yasuaki Okada](#)^{1,2}; ¹Murata Manufacturing Co., Ltd., Japan; ²Pennsylvania State University, United States.

3:30 PM *CM2.2.05
Predicting Materials Strength in BCC Alloys Using Parameter-Less Mesoscale Approaches [Jaime Marian](#); University of California-Los Angeles, United States.

4:00 PM CM2.2.06
Coherent HCP/BCC Interfaces in Zr/Nb Alloys [Maeva Cottura](#); CEA, France.

4:15 PM CM2.2.07
Order Parameter Aided Efficient Phase Space Exploration [Amit Samanta](#); Lawrence Livermore National Laboratory, United States.

SESSION CM2.3: Beyond Atomistic Models II
Session Chair: Chad Sinclair
Wednesday Morning, April 19, 2017
PCC North, 100 Level, Room 125 B

8:30 AM *CM2.3.01
Recent Progress in the Concurrent Atomistic-Continuum Method and Its Applications to Thermal Phonon Transport [Youping Chen](#); University of Florida, United States.

9:00 AM CM2.3.02
A New Implementation of the Concurrent Atomistic-Continuum Method with Quasistatic Algorithms and Mesh Refinement Schemes [Shuozhi Xu](#); Georgia Institute of Technology, United States.

9:15 AM CM2.3.03
Finite-Difference Time-Domain and Monte-Carlo Ray Tracing Hybrid Modeling of Optical Devices and Structures [Mark Portnoi](#); University College London (UCL), United Kingdom.

9:30 AM CM2.3.04
Phase-Field Crystal Model for Ordered Crystals [Eli Alster](#); Northwestern University, United States.

9:45 AM CM2.3.05
Coupling Deterministic and Stochastic Simulations—An Application to Cluster Dynamics in Materials [Pierre Terrier](#); Cermics, Ecole des Ponts, France.

10:00 AM BREAK

SESSION CM2.4: Advance Phase Field Models
Session Chair: Marisol Koslowski
Wednesday Morning, April 19, 2017
PCC North, 100 Level, Room 125 B

10:30 AM *CM2.4.01
On the Incorporation of Environmental Effects in Multi-Scale Modelling Approaches [Esteban P. Bussio](#); ONERA, France.

11:00 AM CM2.4.02
Phase Field Modelling of θ' Precipitation during Aging of Al-4wt.%Cu Alloys—A Multiscale Approach [Javier Llorca](#); IMDEA Materials Institute & Technical University of Madrid, Spain.

11:15 AM CM2.4.03
Modeling Fission Gas Bubble Evolution in Nuclear Fuels with the Phase-Field Method [Larry Aagesen](#); Idaho National Laboratory, United States.

11:30 AM CM2.4.04
Coupling Radiation Damage to Phase Field Microstructure Evolution and Thermal Transport [Larry Aagesen](#); Idaho National Laboratory, United States.

11:45 AM CM2.4.05
Microstructure Evolution of Powder Materials during Solid State Sintering—A Phase Field Study [Sudipta Biswas](#); Purdue University, United States.

SESSION CM2.5: New Developments in Dislocation Dynamics

Session Chair: Esteban Busso
Wednesday Afternoon, April 19, 2017
PCC North, 100 Level, Room 125 B

1:30 PM *CM2.5.01

Residual Stress Predictions in Nanocrystalline Thin Films Marisol Koslowski; Purdue University, United States.

2:00 PM *CM2.5.02

Challenges in Using Spectral Methods for Computing Stress Fields from Dislocations Richard A. LeSar; Iowa State University, United States.

2:30 PM BREAK

3:30 PM CM2.5.03

Modelling Plastic Deformation in Micro- and Nano- Samples Using the Discrete-Continuum Model Riccardo Gatti; LEM UMR 104 CNRS-ONERA, France.

3:45 PM CM2.5.04

A FFT-Based Formulation for Efficient Mechanical Fields Computation in Isotropic and Anisotropic Periodic Dislocation Dynamic Laurent Caplungo; Los Alamos National Laboratory, United States.

SESSION CM2.6: Discrete Dislocation Dynamics I

Session Chair: Benoit Devincere
Wednesday Afternoon, April 19, 2017
PCC North, 100 Level, Room 125 B

4:00 PM *CM2.6.01

Precipitates Strengthening Using Dislocation Dynamics Sylvie Aubry; Lawrence Livermore National Laboratory, United States.

4:30 PM *CM2.6.02

OptiDis—Hybrid MPI/OpenMP Parallelism for Large Scale Dislocation Dynamics Simulations Laurent M. Dupuy; CEA Saclay, France.

SESSION CM2.7: Poster Session

Wednesday Afternoon, April 19, 2017
8:00 PM - 10:00 PM
Sheraton, Third Level, Phoenix Ballroom

CM2.7.01

A Phase-Field Model for the Development of Surface Morphology during Wet Chemical Etching Jin-Ru Miao; National University of Tainan, Taiwan.

CM2.7.02

Computer Simulation of Microstructural Evolution during Oblique Angle Deposition Sheng-Jie Hong; National University of Tainan, Taiwan.

CM2.7.03

3D Micromechanical Modeling of Dual Phase Steels Using the Representative Volume Element Method and Response Surface Methodology: Parametric Study Tarek M. Belgasam; Washington State University, United States.

SESSION CM2.8: Discrete Dislocation Dynamics II

Session Chair: Jaime Marian
Thursday Morning, April 20, 2017
PCC North, 100 Level, Room 125 B

8:30 AM *CM2.8.01

An Anisotropic Non-Singular Theory of Dislocations Giacomo Po; University of California, Los Angeles, United States.

9:00 AM *CM2.8.02

Advanced Time Integration Algorithms for Dislocation Dynamics Simulations of Work Hardening Wei Cai; Stanford University, United States.

9:30 AM *CM2.8.03

Extending the Length and Time Scale of Discrete Dislocation Dynamics by Exploiting Hot-Spot Detection and Grain-Based Parallelization Markus Stricker; Karlsruhe Institute of Technology, Germany.

10:00 AM BREAK

SESSION CM2.9: Discrete Dislocations to Plasticity

Session Chair: Wei Cai
Thursday Morning, April 20, 2017
PCC North, 100 Level, Room 125 B

10:30 AM *CM2.9.01

Influence of Dislocation Cross-Slip and Collinear Annihilation on the Evolution of Dislocation Density and Strain Hardening Benoit Devincere; LEM, CNRS-Onera, France.

11:00 AM CM2.9.02

Developing a Crystal Plasticity Model for Metallic Materials Based on the Discrete Element Method Agnieszka Truszkowska^{1,2}; ¹Oregon State University, United States; ²Oregon State University, United States.

11:15 AM *CM2.9.03

FFT-Based Algorithms for Micromechanical Analysis of Polycrystalline Metals at the Mesoscale Ricardo Lebensohn; Los Alamos National Laboratory, United States.

SESSION CM2.10: Crystal Plasticity

Session Chair: Daniel Weygand
Thursday Afternoon, April 20, 2017
PCC North, 100 Level, Room 125 B

1:30 PM *CM2.10.01

Crystal Plasticity Simulations on Real Data—Towards Highly Resolved 3D Microstructures Martin Diehl; Max-Planck-Institut für Eisenforschung GmbH, Germany.

2:00 PM CM2.10.02

Crystal Plasticity Simulation of Aluminum Lithium Alloy—Verification and Experiments Ali Ramazani; University of Michigan, United States.

2:15 PM *CM2.10.03

Multiscale Modeling of Plasticity Using Data Science Approaches Surya R. Kalidindi; Georgia Institute of Technology, United States.

2:45 PM CM2.10.04

Thermodynamically Consistent and Efficient Phase Field Model for Micro-Elasto-Viscoplasticity Youhai Wen; National Energy Technology Laboratory, United States.

3:00 PM CM2.10.05

Modeling of Dynamic Recrystallization in Austenitic Stainless Steel 304L by Coupling a Full Field Approach in a Finite Element Framework with Mean Field Laws Ludovic Maire; CEMEF Mines ParisTech, France.