

Symposium 8: Defects in Materials

Organizers: Ladislav Kubin, Steve Zinkle, Shahram Sharafat, Hanchen Huang, Anter El-Azab

Oral Presentations

Blue: Keynote presentation (30 minutes)

Black: Invited presentation (20 minutes)

Green: Invited poster presentation

Monday Afternoon (2)

Tomas de la Rubia, Materials, energy and climate: Requirements and strategies for sustainability in the 21st Century

Steve Zinkle, L.M. Wang, Defect cluster patterning in irradiated materials

C.H. Woo, Large-scale spin-lattice dynamics simulation of ferromagnetic iron

Tuesday Morning

Akiyuki Takahashi, Mitsuru Kawanabe, Shotaro Hayashi, Masanori Kikuchi, Nasr Ghoniem, Dislocation dynamics modeling of dislocation cores in the interaction with precipitates

Jaafar El-Awady, Ming Wen, Nasr Ghoniem, The influence of surface ion damage on the mechanical behavior of micro-pillars

Bachu Singh, In-reactor Deformation experiments on FCC and BCC pure metals and alloys

Ladislav Kubin, Benoit Devincere, Thierry Hoc, Scale transitions in the plasticity of f.c.c. single crystals

Michael Zaiser, Size dependence in constrained plasticity: discrete and continuous models of 3D dislocation dynamics

Wednesday Morning

Craig Hartley, Determination of micro-mechanical constitutive relations using dislocation dynamics

Radan Sedlacek, Jan Kratochvil, Cornelia Schwarz, Statistical foundation of continuum dislocation plasticity

Elias Aifantis, Dislocations, gradient theory and nanomechanics

Istvan Groma, Phase field theory of dislocations obtained by coarse graining

Anter El-Azab, A perspective on the development of density-based models of dislocation dynamics

Richard LeSar, Jeffrey Rickman, 3D simulations of evolving dislocation microstructures: connection to coarse graining

Wednesday Afternoon

Talat Rahman, Self learning kinetic Monte Carlo simulations: application to hetero- and homo-epitaxial growth processes

Klaus Schwarz, Anomalous Relaxation in Strained (110) fcc Layers

E.H. Tan, **Lizhi Sun**, Dislocation dynamics simulation in heterogeneous elastic thin films

Mutasem Shehadeh, Sauvik Banerjee, Gang Lu, Nickolas Kioussis, Nasr Ghoneim, The behavior of dislocations in bulk and nano-layered crystals: An ab initio-based parametric dislocation dynamics approach

Thursday Morning

Hanchen Huang, A new characteristic length scale

Garani Ananthakrishna, Tracking acoustic emission and spatial configurations of dislocations during the Portevin-Le Chatelier effect

J. S. Chen, Meshfree Approaches for Modeling Grain Structure Evolution

Javier Gil Sevillano, Mode-II intergranular crack propagation in Cu along a symmetrical tilt boundary

Nicholas Kioussis, Zhengzheng Chen, Nasr Ghoniem, Local chemistry effect on dislocation mobility: sequential and concurrent multi-scale approaches

Thursday Afternoon

Gang Lu, From electrons to finite elements: quantum mechanical simulations at macroscales

Pierre Hirel, Julien Godet, **Sandrine Brochard**, Laurent Pizzagalli, Pierre Beauchamp, Study of dislocation nucleation activation from surface step by atomistic calculations

Catalin Picu, Renge Li, Smooth versus jerky motion of dislocations across fields of obstacles

Michal Benes, Quantitative aspects of microstructure formation in solidification

Zhiqiang Wang, Irene Beyerlein, Richard LeSar, Material deformation under high rate: atomistic, dislocation dynamics simulations and constitutive modeling

Thursday Afternoon (2)

Shahram Sharafat, Akiyuki Takahasy, Koji Nagasawa, Nasr Ghoniem, A description of helium bubble growth in ODS alloys using Monte Carlo simulation

Michael Hribernik, **G. Robert Odette**, Takuya Yamamoto, On the dynamics of cleavage fracture: atomic-dislocation scale mechanisms leading to a universal toughness-temperature shape

S. Bulent Biner, Q. Chen, X-Y Liu, The role of solute segregation on the evolution and strength of dislocation junctions

Poster Presentations

Wednesday Afternoon

1. Xanthippi Markenscoff, **Vassilis Pontikis**, Atomistic study of the core radius of a screw dislocation in bcc-iron
2. **David Rodney**, Laurent Proville, Why is the Peierls stress lower in experiments than in simulations
3. **Michael Anisimov**, Experimental measurements of nucleation rates near critical conditions of binary vapor-gas systems
4. **Vojtech Minarik**, Jan Kratochvil, Karol Mikula, Michal Benes, Advances in numerical simulation of dislocation dynamics
5. **Can Ayas**, Erik van der Giessen, Discrete dislocation dynamics modeling of the relaxation of intrinsic stress in thin films by grain boundary diffusion and plasticity
6. Julien Godet, **Sandrine Brochard**, Tristan Albaret, Laurent Pizzagalli, Atomistic calculations of the formation, stability and mobility of a non dissociated 60° dislocation in silicon
7. **Michel Perez**, Sébastien Garruchet, Coupling molecular dynamics and kinetic Monte Carlo simulations to model the carbon snoek peak in ferrite
8. **Lev Zuev**, Svetlana Barannikova, A new model of plasticity development in solids

9. **Mohamed Chabaat**, Hassène Seddiki, 2D - Stress analysis during the crack-crazing patterns interactions
10. **Silvester Noronha**, Nasr Ghoniem, Garani Ananthakrishna, A dynamical for flow localization in irradiated materials
11. **Nick Kioussis et al.**, Polarization-induced Strengthening Mechanism of Cu Nano-Precipitates in alpha-Fe