

# Agenda for VIIIth CMSN Meeting

October 2-3 Golden Colorado

September 29, 2003

Thursday, October 2nd

7:00-8:00 a.m.

Breakfast at Table Mountain Inn

8:00-8:30 a.m.

*Introduction/Welcome/CMSN issues*

Alain Karma, David Srolovitz

8:30-9:00 a.m.

*Solid-Liquid interfacial energies: FCC vs BCC*

Mark Asta, Northwestern University

9:00-9:30 a.m.

*Solid-liquid interfacial free energies of model systems*

James Morris, Ames Laboratory

9:30-10:00 a.m.

*Atomistic simulations of crystallization rates: Comparison with a result from DFT*

Jeff Hoyt

10:00-10:15 a.m.

Discussions -I

10:15-10:45 a.m.

*Impurity Drag - Relationship between the Cahn model and experiments*

David J. Srolovitz

10:45-11:15 a.m.

*MD simulation on flat tilt grain boundary migration*

Hao Zhang, Mikhail Mendeleev and David J. Srolovitz, Princeton University

11:15 a.m.-11:45 p.m.

*Non-linear grain boundary migration: Theory and simulations*

Moneesh Upmanyu, Colorado School of Mines

A. D. Rollett, Carnegie Mellon University

11:45 a.m. -12:00 p.m.

Discussions -II

12:00-1:00 p.m.

Lunch

1:00-1:30 p.m.

*Phase field modeling of faceted solidification*

Alain Karma, Northeastern University

1:30-2:00 p.m.

*Texturing during directional growth of faceted Si in Al-Si eutectics*

Ralph Napolitano, Iowa State University

2:00-2:30 p.m.

*Dendrite orientation selection*

Tomorr Haxhimali and Alain Karma, Northeastern University

2:30-2:45 p.m.

Discussions - III

2:45-3:15 p.m.

*Competitive growth selection of recrystallization nuclei near hard particles*

Bala Radhakrishnan, ORNL

3:15-3:45 p.m.

*Kinetic Monte-Carlo simulations of nucleation, growth and coarsening in a ternary Ni-Al-Cr alloy*

Zugang Mao and David N. Seidman, Northwestern University

3:45 - 4:00 p.m.

Discussions - IV

4:00-5:30 p.m.

Discussions on future direction, review status, etc..

Friday, October 3rd

7:00-8:00 a.m.

Breakfast at Table Mountain Inn

8:00-8:30 a.m.

*Latest development of bond-order potentials for studies of interfaces and dislocations in BCC transition metals*

Vasek Vitek, University of Pennsylvania

8:30-9:00 a.m.

*Texture evolution during grain growth*

Ning Ma and Yunzhi Wang, Ohio State University

9:00-9:15 a.m.

Discussions - V

9:15-9:45 a.m.

*Equilibrium solid-liquid interfacial solute adsorption in alloys as a function of Lennard-Jones parameters*

Chandler Becker and Mark Asta, Northwestern University

9:45-10:15 a.m.

*Crystal melt interfacial free energy of inverse-power repulsive potentials: Simulations and musings*  
Brian Laird, University of Kansas

10:15 - 10:45 a.m.

*Grain boundary free energy of hard disk assemblies using thermodynamic integration*  
Mark T. Lusk, Colorado School of Mines

10:45 - 11:00 a.m.

Discussions - VI

11:00 - 11:30 a.m.

*Examination of grain boundary mobility in aluminum alloys during recrystallization*  
Mitra Taheri and Tony Rollett, Carnegie Mellon University

11:30 a.m. - 12:00 p.m.

*TBD*

Discussion - VII/Closing remarks/Lunch

List of attendees

Asta, Mark, Northwestern University  
Becker, Chandler, Northwestern University  
Battaile, Corbett, Sandia National Lab  
Depperschmidt, Andy, Colorado School of Mines  
Fellinger, Mike, Colorado School of Mines  
Foiles, Stephen, Sandia National Lab  
Haxhimali, Tomorr, Northeastern University  
Hoyt, Jeff, Sandia National Lab  
Janssens, Koen, Sandia National Laboratory  
Karma, Alain, Northeastern University  
Laird, Brian, University of Kansas (to be confirmed) Lee, Jeehyun, Northwestern University  
Lusk, Mark T., Colorado School of Mines  
Ma, Ning, Ohio State University  
Mao, Zugang, Northwestern University  
Mendelev, Mikhail, Princeton University  
Taheri, Mitra, Carnegie Mellon University  
Morris, James, Ames Lab  
Napolitano, Ralph, Iowa State University  
Radhakrishnan, Bala, ORNL  
Srolovitz, David J., Princeton University  
Trautt, Zachary, Colorado School of Mines  
Upmanyu, Moneesh, Colorado School of Mines Vitek, Vasek, University of Pennsylvania  
Weiland, Hasso, Alcoa  
Zhang, Hao, Princeton University