

This Information can also be found at
neon.mems.cmu.edu/rollett/CMSN.Wkshp5.Agenda.pdf

CMSN Workshop on Anisotropic Boundaries, Solidification and Grain Growth

Where: Center for Theoretical and Computational Materials Science
National Institute of Standards and Technology

When: March 26-27, 2002
Lecture Room E, March 26th
Lecture Room C, March 27th.

Local Host: James Warren (jwarren@nist.gov)

Program point of contact: Tony Rollett, CMU, rollett@andrew.cmu.edu

Start time 9AM

A block of 25 rooms has been set aside at the Gaithersburg Holiday Inn, which will run a shuttle in the morning and evening to the Campus. To reserve a room, call 301-948-8900. The rooms are under the name "CMSN Workshop." The cost is \$99/night. If more rooms are needed, I can get them set aside, but the earlier you book, the better.

Go to http://www.nist.gov/public_affairs/visitor/visitor.htm for information on how to get to NIST.

AGENDA

Tuesday, 26th March, 2002.

9:00am Tony Rollett Opening Remarks

Solid-Liquid Interface Properties

9:15 Ralph Napolitano, Ames: Experimental measurement of crystal-melt interfacial properties.

9:35 Jamie Morris, Ames: Anisotropic properties of crystal-melt boundaries in aluminum.

9:55 Mark Asta, NWU: Calculation of alloy solid-liquid interfacial free energies from atomic-scale simulations.

10:15 Jeff Hoyt, SNL(A): Atomistic Computation of the Kinetic Coefficient for Solidification in the 111 Growth Direction.

11:35 coffee break + discussion

11:00 Alain Karma, NEU: An analysis of higher order gamma-plots with cubic symmetry for phase-field computations of complex dendrite growth morphologies in aluminum alloys.

11:20 Alexander Umantsev: Continuum theory of interfacial segregation: the nonlinear effects.

12:00-1:30 lunch

Properties of Grain Boundaries

1:30 David Saylor, NIST: Integrating Geometric and Crystallographic Statistics in Microstructural Models.

1:50 Hao Zhang and David J. Srolovitz (Presenter HZ), Princeton: Temperature Dependence of Grain Boundary Mobility in 3-D.

2:10 break

2:30 Mikhail Mendeleev and David J. Srolovitz (Presenter MS), Princeton: Fitting Interatomic Potentials to Liquid Structure Data.

2:50 David J. Srolovitz, Mikhail Mendeleev, M. Haataja, and A. Karma (Presenter MS), Princeton: Does Boundary Mobility have a Unique Value?

3:10 Alex Lobkovsky, NIST: TBA.

3:30-? discussion/CTCMS visit/email time

No-host dinner at location TBA

Wednesday, March 27th:

Microstructural Evolution in Solidification

9:00 Ken Jackson: title TBA.

9:20 Daniel Lewis, NIST: 3D Effects in Phase Field Models of Eutectic Growth.

9:50 coffee break + discussion

10:15 Jon Guyer, NIST: Phase Field Modeling of Electrochemistry.

10:35 Julia Slutsker, NIST: Phase Field Modeling of Elastic Domain Structures in Constrained Layers.

10:55-11:30 Discussion

11:30-12:30 Lunch (+ discussion)

Microstructural Evolution in the Solid State

12:30 Corbett Battaile SNL(A): Coupled Simulations of Grain Growth and Deformation.

12:50 Tony Rollett, CMU: Sensitivity of Texture Development to Grain Boundary Energy & Mobility.

1:10 Yunzhi Wang, OSU: Segregation and Phase Transformation at Grain Boundaries.

1:30 B. Radhakrishnan, ORNL: Stored Energy Difference and Abnormal Subgrain Growth.

1:50 Closing discussion

Attending:

Jeff McFadden

Ning Ma

Kee-Young Jung

David Kinderlehrer

Irene Livshits

Dale Koelling

Leiser, Manfred

Chuck Romine

Jeehyun Lee

Deyan Sun

Hasso Weiland

H. Harriet Kung

Priya Manohar

Mark Locatelli

