

CMSN Coordination Meeting
Oak Ridge National Laboratory
March 18-19, 2004

Meeting Schedule

March 18

8:30 – 9:00 AM – opening remarks (Tony Rollett, Alain Karma, Thomas Schulthess, James Morris)

9:00 – 9:30 AM – Jim Roberto, Associate Laboratory Director, Physical Sciences, ORNL.

9:30 – 9:55 AM - Modeling the Motion of Theta-Prime/Matrix Interfaces in Al-Cu, L-Q. Chen, Penn State

9:55-10:20 AM - Dendrite Growth Orientation Selection: Beyond Extremal Principles, Tomorr Haxhimali

10:20-10:35 - Break

10:35 – 11:00 AM - Effect of non-equilibrium vacancy concentration on grain boundary motion in Au, Moneesh Upmanyu and Branden Kappes, CSM.

11:00 – 11:25 AM - Effect of Fe Impurities on Grain Boundary Motion in Al, M.I. Mendeleev, D.J. Srolovitz, S. Han, G.J. Ackland, J.R. Morris

11:25 – 11:50 AM - Effect of Normal-dependent Grain Boundary Energies on Population Statistics, Jason Gruber, Greg Rohrer and Tony Rollett, Carnegie Mellon

11:50 AM – 12:45 PM – Lunch

12:45 – 1:10 AM - "The Effect of Inclination on Grain Boundary Mobility" Hao Zhang, Mikhail I. Mendeleev and David J. Srolovitz

1:10 PM – 1:35 PM - The mechanisms of coarsening of the gamma prime phase in Ni-Al-Cr alloys via kinetic Monte Carlo simulations, Zungang Mao and D.N. Seidman, Northwestern University

1:35 – 2:00 PM - Coupled Growth in Eutectic and Peritectic Alloys: New Insights from Phase-Field Modeling and Experiments, Alain Karma, North Eastern University

2:00 – 2:25 PM - Studies of the effect of solute on grain boundary mobility and character in Al alloys, Mitra L. Taheri and Tony Rollett, Carnegie Mellon

2:25 – 2:50 PM - Growth mechanisms and impurity effects in Al-Si, Ralph Napolitano, Iowa State

2:50 – 3:15 PM - A comparison between Kinetic Monte Carlo simulation and three-dimensional atom-probe microscopy results on a Ni-Al-Cr alloy, D.N. Seidman, Northwestern University

3:15 – 3:30 PM - Break

3:30 PM – 5:30 PM – Discussions (Separate Sessions for S-S and S-L interface groups)

March 19

8:30 – 9:00 AM – Thomas Zacharia, Associate Laboratory Director, Computing and Computational Sciences Directorate, ORNL

9:00 – 9:25 AM - Equilibrium Solution Thermodynamics and Solid-Liquid Interfacial Adsorption in Lennard-Jones Alloys, C.A. Becker and M. Asta, Northwestern University

9:25 – 9:50 AM - Phase field modeling of defect mediated growth, Jim Warren, NIST

9:50 – 10:05 Break

10:05 – 10:30 AM - Effect of solute drag on the evolution of polycrystalline microstructures, N. Ma, S. A. Dregia and Y. Wang, Ohio State

10:30 – 10:55 AM - Density Wave Theory of the fcc-liquid Interface Anisotropy, Kuo-An Wu

10:55-11:20 AM - Progress in 3D computational modeling of solute diffusion during microstructure evolution, Koenraad G. F. Janssens, Sandia National Laboratories

11:20 – 11:45 – Phase-field modeling of solidification, M. Plapp, Ecole Polytechnique,

11:45 – 1:00 PM - Wrap up, Lunch