CMSN Research Team: "Fundamentals of Dirty Interfaces"

Meeting Agenda: November 1-2 2005, Santa Fe NM

Tuesday November 1 2005

Solid-Solid Interface Properties

08:30am – 09:00am	J. Gruber, G.S. Rohrer, and A.D. Rollett, "Grain Boundary Populations versus Boundary Anisotropy"
09:00am – 09:30am	K.G.F. Janssens, E.A. Holm, S.M. Foiles, and D. Olmsted, "Mobility of Flat Grain Boundaries Under a Synthetic Driving Force"
09:30am – 10:00am	M. Upmanyu, Z.T. Trautt, B. Kappes, H. Liang, and A. Karma, "Absolute Grain Boundary Mobility from Boundary Plane Random Walk: Near Equilibrium Calculations"
10:00am – 10:15am	**Break**
10:15am – 10:45am	Z.T. Trautt, M. Upmanyu, B. Kappes, H. Liang, and A. Karma, "Grain Boundary Stiffness Depends on Stored Energy of Deformation"
10:45am – 11:15am	H.-S. Nam, M.I. Mendelev and D.J. Srolovitz , “Liquid Metal Embrittlement of Grain Boundaries in Binary Alloys: The Role of Grain Boundary Diffusion”
11:15am – 11:45am	J.E. Guyer, D. Wheeler, and J.A. Warren, "Solving PDEs with FiPy"
11:45am – 01:30pm	**Lunch**

Solid-Solid Interface Motion

01:30pm – 02:00pm	M.I. Mendelev, H. Zhang, D.J. Srolovitz, and J.R. Morris, "Comparison of Grain Boundary and Solid-Liquid Interface Migration in FCC Metals"
02:00pm – 02:30pm	M. Gao, J. Gruber, and A.D. Rollett, "Combined Finite Element and Finite Diffusion Modeling of Solute Drag in Grain Growth"
02:30pm – 03:00pm	A. Caro, D. Farkas, E. Bringa, G. Gilmer, L. Zepeda-Ruiz, and B. Sadigh, "Ultra Hard Nanophase Materials under Shock Loading and the Influence of Impurities in GB Motion"
03:00pm – 03:15pm	**Break**
03:15pm – 03:45pm	N. Brown, N. Ma, Y. Wang and S.D. Dregia, "Polydomain Coarsening: Geometrical, Topological, and Statistical Effects"
03:45pm – 04:15pm	B. Radhakrishnan, "Large-scale 3-D Simulations of Zener Drag"
04:15pm – 04:45pm	B. Kappes, M. Upmanyu, Z.T. Trautt, H. Liang, and A. Karma, "Grain Boundary - Pore Interactions"
04:45pm – 05:00pm	**Break**
05:00pm – 05:30pm	N. Ma, N. Zhou and Y. Wang, "Effect of Texture and Precipitates on Grain Growth: Quantitative Phase Field Modeling with Experimental Micrographs as Input"
05:30pm – 06:00pm	Z. Mao, G. Martin, and D.N. Seidman, "The Effects of Solute-Vacancy Binding Energies on Coarsening Mechanisms in a Model Ni-Al-Cr Superalloy via Lattice Kinetic Monte Carlo Simulations"

Wednesday November 2 2005

Solid-Liquid Interface Properties

08:00am – 08:30am	K.-A. Wu and A. Karma, "Phase-Field Crystal Free-Energies for Crystal Structures that Matter"
08:30am – 09:00am	C.A. Becker, M. Asta, J.J. Hoyt, S. M. Foiles, and D. Olmsted, "Solid-Liquid Interfacial Free Energies in Binary Lennard-Jones Alloys"
09:00am – 09:30am	B.B. Laird, X. Feng, and M. Amini, "Crystal-Melt Interfacial Properties via Simulation: The Interfacial Free Energy of Succinonitrile and the Kinetic Coefficient of Hard-Spheres"
09:30am – 09:45am	**Break**
09:45am – 10:15am	J.R. Morris, R.S. Aga, J.J. Hoyt, and M. Mendelev, "Using Crystal-Melt Interfacial Free Energies to Predict Nucleation Rates"
10:15am – 10:45am	T. Haxhimali, A. Karma, M. Asta, and J.J. Hoyt, "Growth Directions of Dendritic Crystals with Hexagonal Symmetry"

Solid-Liquid Interface Motion

10:45am – 11:15am	D. Buta, M. Asta, and J.J. Hoyt, "Simulations of Crystal Growth at Stepped Solid-Liquid Interfaces of Stillinger-Weber Silicon"
11:15am – 11:45am	J.J. Hoyt, "Effect of Stress on Melting and Freezing in Nanopores"
11:45am – 01:30pm	**Lunch**
01:30pm –	**Discussion and Administrative Business**