Northwestern | McCORMICK SCHOOL OF ENGINEERING
Materials Science and Engineering

DOW Lecture

David Srolovitz

Professor
Engineering and Applied Science
Director of the Penn Institute for Computational Science
University of Pennsylvania

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"Grain-Boundary Metastability and its Statistical Properties"

Grain-boundary (GB) structure and properties are usually analyzed in terms of ground-state (minimum-energy) GB states. However, global equilibrium is rarely achieved in materials. I will discuss the nature of GB metastability and its impact on material properties. Higher-energy GB states can be the result of nonequilibrium processes or simply thermal excitations. While the existence of limited GB metastability is widely known for a few simple GBs, I demonstrate that the multiplicity of metastable GB states is, in general, very large. This conclusion is based upon extensive atomistic bicrystal simulations for both symmetric tilt GBs and twist GBs in three very different materials. The energies of these GB states are densely distributed so that the dependence of the GB energy on misorientation is better described as an energy band rather than as a single curve as in the traditional picture. Based upon the distribution of metastable GB states, I introduce a GB statistical-mechanics picture and apply it to predict finite-temperature equilibrium and non-equilibrium properties. When GB multiplicity exists, GB structures can be thought of as domains of different GB states separated by various classes of line defects. The existence of a large set of metastable GB states, very close in energy, suggests an analogy between the behaviors of GBs and glasses and implies the potential for GB engineering. (N.B. - this presentation is complementary to that presented in April at Northwestern as part of the Midwest Mechanics Seminar.)

Biography: David Srolovitz is the author of well over 450 papers on topics in materials theory and simulations ranging from defects (surfaces, grain boundaries, dislocations, point defects), microstructure evolution (grain growth, dislocations, stress effects, phase transformations), deformation (nanomaterials, dislocation motion, creep), and film growth (sputtering, evaporation, CVD) and has an *h*-index of 75 with more than 20,000 literature citations. He is a Member of the National Academy of Engineering, Fellow of MRS, TMS, ASM, Institute of Physics and is the winner of the 2013 MRS Materials Theory Award. Srolovitz did his undergraduate work in Physics at Rutgers University and PhD from the University of Pennsylvania. He was a staff member at Exxon Corporate Research and Los Alamos National Laboratory early in his career and then was professor at the University of Michigan (Materials Science and Applied Physics), Princeton University (Mechanical and Aerospace Engineering, Applied Mathematics), and the University of Pennsylvania (Mechanical Engineering and Applied Mechanics), where he is currently the Joseph Bordogna Professor of Engineering and Applied Science and Director of the Penn Institute for Computational Science.