Carnegie Mellon
Materials Science and Engineering Seminar Series
Richard LeSar
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Iowa State University

"*Theory and Simulation of Dislocation Structure and Response*"

Friday, September 7, 2007
11:00 A.M. Seminar in The Singleton Room

Despite 70 years of effort since the introduction by Taylor and Orowan of dislocations to describe deformation in metals, much remains to be learned about how dislocation microstructures form and how they affect materials response. We will describe recent advances in the simulation of dislocations, focusing on deformation in *fcc* metals at high strain rates. We will also discuss the limitations of discrete dislocation dynamics methods and the need for descriptions of deformation based on coarse-grained representations of dislocation structures. To that end, we will present recent results on scaling relations that couple structures across scales as well as some interesting experimental and simulation results that indicate that dislocations show self-organized response, much like earthquakes.

Richard LeSar is professor and chair of the Department of Material Science and Engineering at the Iowa State University. He arrived at Iowa State in the summer of 2006 after many years as a staff member at the Los Alamos National Laboratory. He received his BS in Chemistry from the University of Michigan, and his AM and PhD from Harvard University. Richard LeSar's work focuses on the development and application of theory, modeling, and simulation of materials structures and properties. He has interest in modeling at many scales, with recent applications of electronic structure calculations (perovskites), atomistic simulations (molecular and metallic systems) and mesoscale simulations (dislocation dynamics). His work is currently focused in the areas of employing dislocation simulations to guide the development of new theories of plasticity and development of coarse-grained descriptions of biomolecules for simulating large-scale molecular processes.