Georgia Institute of Technology
The George W. Woodruff School of Mechanical Engineering

Woodruff Colloquium

"Multiscale Modeling in Materials and Mechanics"

Professor William Curtin
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Tuesday, January 16, 2007
MARC Building Auditorium
11:00 a.m.

Abstract **:**

Mechanical phenomena such as crack growth (by high loading, fatigue, or chemical embrittlement), dislocation nucleation, and grain boundary deformation, all require explicit retention of nanoscale details but are also strongly influenced by, for instance, dislocations and their motion (plasticity) at the micron and larger scales. Efficient, accurate calculations of such material behavior rely on multiscale methods to reduce the number of degrees of freedom in any computation.

To handle multiple scales simultaneously, the Coupled Atomistic and Discrete Dislocation (CADD) method is introduced wherein atomistic and continuum regions communicate across a seamless boundary and exchange dislocations back and forth as dictated by the mechanics of the problem. The atomistic region can experience any deformations that occur under the applied loading while the continuum region evolves according to discrete dislocation plasticity. Comparisons of CADD against full atomistic simulations validate the method. Applications to nanoindentation and dislocation/grain-boundary interactions are then presented. The extension of the method to include finite-temperature dynamics in the atomistic region is demonstrated, and applied to predict crack-tip dislocation emission.

The general concepts developed here also motivate the formulation of new multiscale models at other scales. Examples include coupling discrete dislocations to continuum crystal plasticity, coupling discrete kinetic Monte-Carlo models of diffusion to continuum diffusion, coupling quantum mechanics to continuum models, and new discrete dislocation models for polycrystals and bimaterial interfaces. Collectively, these multiscale models can be used to study a wide range of issues in the design of structural and electronic materials.

Biographical Sketch:

Dr. William Curtin received his Ph.D. in theoretical physics from Cornell University in 1986 and joined the British Petroleum Research Laboratories in Cleveland, OH. Between 1993 and 1998, he was on the faculty at Virginia Tech. Since 1998, he has been a Professor at Brown University and is currently the Elisha Benjamin Andrews Professor.

Professor Curtin's current research focuses on multiscale modeling of the mechanical behavior of materials, with specific applications to fiber composites, atomistic/continuum models of plasticity and fracture, solute hardening in aluminum alloys, impurity/defect diffusion, carbon-nanotube-based ceramic composites, electrical sensing of damage in polymer composites, and mechanics of complex microstructures.

Dr. Curtin is Director of the Center for Advanced Research Materials and Director of the NSF Materials Research Science and Engineering Center at Brown. He was appointed as a Guggenheim Fellow in 2006, has published over 125 technical papers, and has presented many invited talks at national and international venues.

Refreshments will be served.

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