Nonlinear Multiscale Modeling of Polymer Materials

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Polymer nanocomposite materials have the potential to provide significant increases in mechanical properties relative to current polymers used for structural applications, such as high-performance polymers used in aerospace vehicles. To facilitate the development of polymer nanocomposite materials, constitutive relationships must be established that predict the bulk mechanical properties of the materials as a function of the molecular structure. One promising approach to establishing structure-property relationships of nanostructured materials is to use multiscale modeling techniques. Molecular Dynamics (MD) simulations can be used to predict the equilibrated molecular structure of a material and to predict the behavior of the molecular system when subjected to applied deformations. Although this type of approach is routinely performed on material systems that consist of crystalline atomic structures, little is known on how to apply these techniques on amorphous, organic materials systems, such as polymers and polymer nanocomposites.

The talk will address a multiscale modeling method that has been recently developed to predict bulk-level properties of polymers and polymer composites based on molecular structure. The mechanical properties of several polymer-based systems have been determined as a function of atomic potential, temperature, and model size. These results have been used to predict the behavior of aerospace structures at NASA Langley Research Center.

Greg Odegard earned his B.S. in Mechanical Engineering at the University of Colorado at Boulder in 1995. He earned an M.S. in Mechanical Engineering and a Ph.D. in Engineering at the University of Denver in 1998 and 2000, respectively. From 2000-2002 Prof. Odegard was a National Research Council Research Fellow at NASA Langley Research Center in Hampton, VA. In 2002 he became a staff scientist at the NASA-based ICASE, and continued to work at NASA Langley Research Center from 2003 to 2004 as a staff scientist at the National Institute of Aerospace. In the fall of 2004, Prof. Odegard joined the faculty in the Department of Mechanical Engineering - Engineering Mechanics at Michigan Technological University in Houghton, MI. He has taught classes in Continuum Mechanics and Fracture Mechanics. His research interests include the multiscale modeling and simulation of various materials including nanostructured materials, electroactive materials, structural foam materials, and skeletal muscle tissue.

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