# AEROSPACE & MECHANICAL ENGINEERING

## 2004 COLLOQUIUM 2005

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**UNIVERSITY OF NOTRE DAME, NOTRE DAME, INDIANA 46556**

### *MIDWEST MECHANICS SEMINAR*

**SPEAKER:** **Professor Mary C. Boyce**
Department of Mechanical Engineering
Massachusetts Institute of Technology
Cambridge, Massachusetts

**TOPIC:** **MECHANICS OF THE FINITE DEFORMATION BEHAVIOR OF BIOMACROMOLECULAR NETWORKS**

**DATE:** Tuesday, February 22, 2005

**TIME:** 3:30 p.m.

**PLACE:** 138 DeBartolo Hall

### *ABSTRACT*

The force-extension behavior of many biomacromolecules is known to exhibit a characteristic repeating pattern of a nonlinear rise in force with imposed displacement to a peak, followed by a significant force drop upon reaching the peak (a "saw-tooth" pattern) due to stretch-induced unfolding of modules along the molecular chain. This behavior is speculated to play a governing role in the function of biological materials and structure. In this paper, models for the mechanical behavior of single modular macromolecules and networks of such macromolecules are developed enabling understanding of the manner in which this characteristic single molecule behavior is translated to the behavior of molecular strands, membranes, and solids. Single molecule force-extension behavior is modeled using the Freely-Jointed Chain and Worm-Like Chain models of statistical mechanics together with a new unfolding criterion based on the orientation distribution of folded modules. The single molecule behavior is then used within a continuum mechanics framework to construct constitutive models of the finite deformation stress-strain behavior of two- and three-dimensional networks of modular biomacromolecules. The proposed planar network model has applicability to biological membrane skeletons and the three-dimensional network model emulates cytoskeletal networks and solid biological tissues containing modular macromolecules. Simulation of the multiaxial stress-strain behavior of these networks illustrates the macroscopic membrane and solid stretching conditions which activate unfolding in these microstructures. The models simultaneously track the evolution in underlying microstructural features with different macroscopic stretching conditions, including the evolution in molecular orientation and the number of folded and unfolded modules. One role of this behavior in biological materials is illustrated in a study of the tensile deformation of nacre where the unfolding behavior of the organic matrix molecules is found to mitigate load transfer to the mineral tablets and thus provide enhanced strain to failure and toughness of the biocomposite nacre material over that of the bulk mineral.

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**NOTE:** ***If you are interested in meeting individually with Prof. Boyce, please contact Evelyn at 631-5431.***