NU Mechanical and Industrial Engineering Colloquium Series – FALL 07
WEDNESDAY Sept 19, Room 206 Egan

PROGRAM

12:30 - 1:00 p.m. Pizza/refreshments
1:00 - 1:50 p.m. Lecture (typical)
1:50 - 2:00 p.m. Q&A and Discussion

ABSTRACT

Proteins constitute critical building blocks of life, forming biological materials such as hair, bone, skin, spider silk or cells, which play an important role in providing key mechanical functions in biological systems. However, the fundamental deformation and fracture mechanisms of biological protein materials remain largely unknown, partly due to a lack of understanding of how individual protein building blocks respond to mechanical load. Such models are vital to advance models of diseases, the understanding of biological processes such as mechanotransduction, or the development of biomimetic materials. Here we use large-scale molecular dynamics (MD) simulations combined with statistical theories to develop predictive models of the deformation and fracture behavior of protein materials. We derive a theoretical model that explicitly considers the hierarchical architecture of proteins, including the details of their chemical bonding, capable of accurately predicting their unfolding behavior and thereby providing a rigorous structure-property relationship. We exemplify the approach in the analysis of the deformation mechanisms of beta-sheets and alpha-helices, two prominent protein motifs that form the basis of many protein materials, including spider silk and intermediate filaments. Spider silk is a protein material that can reach the strength of steel cables, despite the predominant weak hydrogen bonding. Intermediate filaments are an important class of structural proteins responsible for the mechanical integrity of eukaryotic cells, which, if flawed, can cause serious diseases such as the rapid aging disease *progeria* or muscle dystrophy. For both examples, our studies elucidate intriguing material concepts that enable to balance strength, energy dissipation and robustness by selecting nanopatterned, hierarchical features.

SEMINAR TITLE

"Hierarchical nanomechanics of protein materials: Robustness, strength and adaptability"

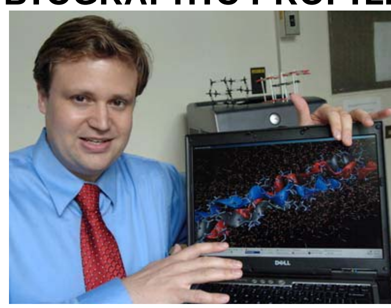
SEMINAR SPEAKER

Professor Markus Buehler,
Esther and Harold Edgerton Assistant Professor

Department of Civil Engineering

MIT

BIOGRAPHIC PROFILE



After obtaining his undergraduate education at the University of Stuttgart, Germany in Chemical and Process Engineering, Prof. Buehler received his M.S. degree in Engineering Mechanics from Michigan Technological University, in 2001. From 2001 to 2004 he worked at the Max Planck Institute for Metals Research in Stuttgart, Germany as a research assistant from where he also received his Ph.D. in Chemistry. From 2004 to 2005, Prof. Buehler was the Director of Multiscale Modeling and Software Integration at the Materials and Process Simulation Center at Caltech, overseeing multiscale method development and applications in modeling of small-scale materials phenomena. In 2005, he joined Massachusetts Institute of Technology (MIT) in the Department of Civil and Environmental Engineering. He founded MIT's Laboratory for Atomistic and Molecular Mechanics, where his research is focused on multi-scale modeling of complex hierarchical protein materials. He is currently the associate editor of the Journal of Computational and Theoretical Nanoscience and guest editor of the Journal of Materials Science. He has made significant contributions in the field of atomistic and molecular modeling of deformation and fracture of brittle, ductile and biological materials. His research has been highlighted in several journals, including the MIT Technology Review, New Scientist and Materials Today. Prof. Buehler has been awarded the 2004 Materials Research Society Gold Graduate Student award and the 2007 National Science Foundation CAREER award. He has recently been invited to join the Frontiers of Engineering Symposium of the U.S. National Academy of Engineering, and will be a keynote speaker at the 2nd Conference on Mechanics of Biomaterials and Tissues in 2007.

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