



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

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Proteins constitute critical building blocks of life, forming various biological materials that play an important role in providing key mechanical functions in biological systems. 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. However, such understanding is vital to advance models of diseases, the understanding of biological processes such as mechanotransduction, or the development of biomimetic materials. Recent theoretical and computational progress provides us with the first insight into such mechanisms and clarifies for the first time how biology 'works' at the molecular scale, and how this relates with macroscopic phenomena such as cell mechanics or tissue behavior, across multiple hierarchical scales. Here we review how molecular dynamics (MD) simulations implemented on ultra-large computing facilities, combined with statistical theories, is used to develop predictive models of the deformation and fracture behavior of protein materials. This approach 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.

Markus Buehler obtained his undergraduate education at the University of Stuttgart in Chemical and Process Engineering, received his M.S. degree in Engineering Mechanics from Michigan Tech in 2001 and earned his PhD in Chemistry from the Max Planck Institute for Metals Research in Stuttgart, Germany in 2004. After an appointment as the Director of Multiscale Modeling and Software Integration at the Materials and Process Simulation Center at the Cal Tech he joined MIT in 2005 as a Postdoctoral Associate, and in 2006 he became a faculty member in MIT's Department of Civil and Environmental Engineering. Prof. Buehler founded MIT's Laboratory for Atomistic and Molecular Mechanics, where his research has pioneered the multi-scale analysis of deformation and fracture of biological protein materials. Prof. Buehler has received several awards, including the 2004 Materials Research Society Gold Graduate Student award, the 2007 National Science Foundation CAREER award, and the 2008 U.S. Air Force Young Investigator Award. He currently holds the Esther and Harold E. Edgerton Career Development Professorship at MIT.