INTEGRATING MECHANICS AND CHEMISTRY: PLASTICITY AND FRACTURE OF PROTEIN-BASED MATERIALS

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Abstract:

The structure and behavior of proteins plays an overarching role in determining their function in biological systems. In recent years, proteins have also been proposed as basis for new materials to be used in technological applications [1]. However, up to date little understanding exists about the atomic and molecular scale deformation mechanisms of protein-based materials. Our goal is to understand the macroscopic mechanical response of chemically complex biological materials based on their fundamental, atomistic ultrastructure using large-scale, massively parallelized modeling techniques. Here we focus on the mechanics of proteins and protein crystals, serving as model systems for other, more complicated biological materials. It is known that protein crystals show quite interesting mechanical behavior, as some of them are extremely fragile, while others can be quite sturdy. However, unlike other crystalline materials like silicon or copper, the mechanical properties of protein crystals have rarely been studied by atomistic computer modeling. As a first step towards more fundamental understanding of the mechanics of those materials, we report atomistic studies of mechanical properties of protein crystals using empirical potentials focusing on elasticity, plasticity and fracture behavior. Here we consider two proteins, Lysozyme, a well-studied enzyme, as well as a small protein α-conotoxin PnIB from *conus pennaceus*. We use large-scale atomistic simulations to determine the low-strain elastic constants for different crystallographic orientations. We also investigate the large-strain elastic properties including plastic deformation. Furthermore, we perform systematic studies of the effect of mutations on the elastic properties of the protein crystal. Our results indicate a strong impact of mutations on elastic properties, showing the potential of mutations to tailor mechanical properties [2]. We conclude with a study of mode I fracture of protein crystals, relating our atomistic modeling results with Griffith's theory of fracture. Finally, we demonstrate our new concept of reactive potentials for modeling protein based materials. Reactive potentials allow first principles based study of formation and breaking of chemical bonds, while being computationally feasible to treat systems with more than 10,000 atoms. We apply the new techniques to investigate the unfolding mechanics of proteins. Our results of force-displacement curves differ significantly from classical modeling attempts with nonreactive potentials such as CHARMM or AMBER, but agree well with experiment. This demonstrates the importance of chemistry in determining the large-deformation mechanics of protein-based materials.

References:

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2. Buehler, M.J., *Atomistic modeling of elasticity, plasticity and fracture of protein crystals.* Submitted to: Model. Sim. Mat. Science and Engr., 2005.

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