Atomistic and continuum modeling of collagen: Elasticity, fracture and self assembly

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One of the emerging frontiers in theoretical and applied mechanics is the development of understanding of the fracture and deformation behavior of chemically complex materials. Many biological materials belong to that class of materials, as they show great chemical and structural complexity, often ranging throughout many hierarchies of scales. However, a thorough theoretical understanding of the deformation mechanics of many biological materials remains elusive up to date. Here we report studies of the mechanical properties of collagen, ranging from the atomistic to the continuum scale. We investigate the mechanics of individual tropocollagen molecules under different types of mechanical loading including tension, compression, shear and bending. Our modeling yields predictions of the fracture strength of single tropocollagen molecules, polypeptides, and also enables quantifying the interactions between tropocollagen molecules. Atomistic modeling predicts a persistence length of tropocollagen molecules $\xi \approx 23.4$ nm, close to experimental measurements. Our studies suggest that in order to describe large-strain or hyperelastic properties, it is critical to include a correct description of the bond behavior and breaking processes at large bond stretch, information that stems from the quantum chemical details of bonding. We use this series of full atomistic calculations to derive parameters for a mesoscopic bead-spring model of tropocollagen molecules. We demonstrate that the mesoscopic model enables studying the finite temperature, long-time scale behavior of tropocollagen fibers, as well as the dynamics of assemblies of individual tropocollagen molecules in fibrils, over time scales approaching microseconds. Using the mesoscopic model, we discover that tropocollagen molecules with high aspect ratio undergo a self-folding mechanism, assembling into nano-rings and small racket-like structures. We also find that fibril-like structures under compression undergo a helical transformation under increasing mechanical load.

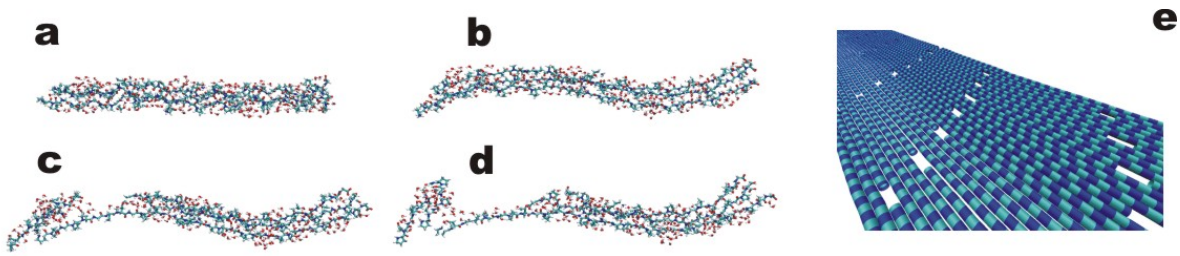

Figure: Hierarchical multi-scale modeling of the mechanical properties of collagen. Subplots (a)-(d) show modeling results using a reactive potential, enabling studying the fracture behavior of individual tropocollagen molecules, while incorporating the chemical complexity of bond breaking and formation. The information obtained from full atomistic modeling is then used to derive parameters for a mesoscopic model, which enables to reach much higher length and time scales. Subplot (e) shows the molecular mesoscale model of a fibril-like structure [1].

[1] M.J. Buehler, "Atomistic and continuum modeling of mechanical properties of collagen: Elasticity, fracture and self-assembly", submitted to: *Journal of Materials Research.*