NATURE DESIGNS COLLAGEN TO RESIST BRITTLE FRACTURE: A CRITICAL LENGTH SCALE FOR TOUGH FIBRILS

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Molecular dynamics (MD) is a powerful tool to understand the mechanics of materials from a fundamental viewpoint. Here we present development of new atomistic and molecular models capable of describing the mechanical properties of chemically complex hierarchical biological materials, bridging atomic and macroscopic scales. We focus on the mechanics of collagen, a protein-based material with superior mechanical properties. Collagen consists of fibrils that are composed of a staggered array of ultra-long tropocollagen molecules with extremely large aspect ratio. We report atomistic and molecular studies focusing on the fracture mechanics of individual tropocollagen molecules and collagen fibrils based on ReaxFF reactive force fields. Theoretical and molecular modeling suggests that the natural design of collagen fibrils maximizes use of covalent bonding in tropocollagen molecules under deformation, while allowing for increased energy dissipation, thus creating a tough and robust material [1]. We discover a critical length scale L_χ characterizing the length of tropocollagen molecules at which deformation of collagen fibrils change from ductile-like shear to brittle-like rupture of molecules. We find that the strength and energy dissipation is maximized as the length of tropocollagen molecules approaches L_χ. First principles based atomistic modeling of the fracture and shear properties of tropocollagen molecules yield a critical length scale L_χ between 290 and 436 nm. Our results suggest that nature designs collagen to resist brittle fracture by selecting tropocollagen molecules at this critical length scale. Our hypotheses are confirmed by large-scale molecular modeling of collagen fibrils comprising of several hundred tropocollagen molecules. Our results help to explain why tropocollagen molecules in Nature are found with lengths in the proximity of 300 nm.

References:

[1] M.J. Buehler, “Nature designs collagen to resist brittle fracture: A critical length scale for tough fibrils”, under submission.

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