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Water Effect on Mechanical Properties of Silk Fibroin

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Silk has been a centuries-old textile material which possesses outstanding mechanical properties. *Bombyx mori* silk (silkworm silk) fibroin structure is composed of hydrophobic nanocrystal domains and hydrophilic amorphous domains. In this study, we perform tensile test and pull-out test on nanocrystal β-sheets to investigate the mechanical property of *Bombyx mori* silk fibroin in explicit water solvent via molecular dynamics simulation. The rupture force for pulling out a β-sheet strand from a nanocrystal lattice is strand-position-dependent. Temperature also plays an important role in determining the mechanical properties of silk fiber.
Mechanical behavior of silk fibroin in vacuum is also investigated. It is found that young's modulus of silk nanocrystal domain in water solvent is lower than that in vacuum. Water molecules could break the hydrogen bonds in between beta-sheets. Our study provides great implications for understanding the mechanical properties and design of silk-based novel materials.

Keywords: Silk fibroin, molecular dynamics, water effect