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PROCEEDINGS

Unique Mechanism in Strength and Deformation of Natural Nano-Sized Fibers: Molecular Dynamics Study on Nanofibrils of Cellulose and Spider Silk

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ABSTRACT

Natural nanofibers, e.g., cellulose nanofiber (CNF) of plant, collagen fibril in human body and fibroin fiber in spider silk, show interesting and distinctive atomistic mechanisms in deformation under mechanical loading as well as exhibition of extraordinary strength. These fibers are comprising more larger bulk and wire materials by constructing structural hierarchy. However, the initiation of unique behavior of these materials largely originates from atomic-scale and chemical energetics in loading. Besides, the experimental approach is often difficult and is too limited to reveal the basic mechanism. Therefore, it is crucial to clarify atomic behavior of these natural nanofibers by theoretical computer modeling and simulation. In this study, first, all-atomic model of CNF was made and it was subject to elastic and plastic deformation by using molecular dynamics (MD) method, which is conducted with force fields applicable for these polymers. Young's moduli and fracture behavior of single CNF were assessed. Subsequently, a computation model of multiple CNFs is built and shear and lubrication mechanisms in contacting and sliding each other were evaluated. It is concluded that the effect of water environment was remarkable. Next, as naturally existing fibers, a couple of short and molecular units found in spider silk nanofiber (SSNF) were computationally reproduced by connecting several existing peptide substances, and realistic MD models of fibrous protein were formed. These fibers which mimic natural SSNF were applied a longitudinal stretch. It was found that they showed a kind of super-elasticity. Cyclic loading tends to give irreversible change in conformation of SSNF and it also leads to deterioration of the molecular structure. It was suggested that the ductility and strength of SSNF are extraordinary and unique in atomic scale.

KEYWORDS

Nanofibril; cellulose nanofiber; spider silk; molecular dynamics; all-atom model; elasticity; plasticity; water; strength

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