

Mechanical modeling and simulation of collagen fibers and fibrils: microscopic deformation mechanism caused by spiral structure

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Abstract

Collagen is one of important proteins in animal body. It is well known that hard tissues, such as bone, tendon and cornea, comprise collagen fibers and fibrils (with other supporting substances), though the structure contains lots of hierarchical stages. From the perspective of structural biology or materials science, the relation between structure and deformation mechanism of collagen is interesting and should be well studied. In this study, we are conducting a molecular dynamics (MD) simulation of collagen structures from atomic scale. The characteristic feature of microscopic collagen is that its single molecule is built up with a triple-helical conformation which is called "tropocollagen(TC)." The TC structure is computationally reproduced just based on the internationally popular database, PDB (protein data bank) . Following the former MD study [Buehler(2008)] which applies the coarse-grained spring-beads model, we construct a long fibrous chain of TC molecule and its aggregated bundle (usually called "fibril") models. The total length of TC models is that of real collagen fibers (approximately 300 nm). To mimic a firm intermolecular bonding, a potential function for the cross-link (CL) points is included in the form of a Lennard-Jones potential with an augmented energy parameter, as well as intramolecular (stretch and bending, but excluding torsion) potentials. The largest number of TCs in a fibril is 16. In order to study mechanical properties, a tensile or a compressive testing is configured with periodic boundary condition in the fiber direction and is dynamically simulated.

The stress-strain (SS) curve is obtained in tensile loading and Young's modulus of the fibril is calculated. It is found that the modulus value depends on the number of TC fibers. In high temperature case, the stiffness tends to decrease remarkably. The yield stress of fibrils increases with increase of the number of TCs, because each CL bonds tends to delay locally a plastic and permanent deformation.

In compressive loading, the SS curve is also obtained, where a sudden drop of stress is detected and it is supposed to be a buckling behavior. The buckling of TC fibrils occurs not in a whole structure but at individual binding sites of CL separately.

The degree of microscopic spiral (triple helix) inherent in TC conformation affects both stiffness (Young's modulus) and buckling stress of TC fibril. Consequently, we conduct loading simulations for several TC fibril models with a different orientation angle (it is the angle between the oblique molecular direction and the axial loading direction) [Shirahana(2015)]. The smaller the orientation angle is, the larger the strength, Young's modulus or the buckling stress is obtained. It is reasonably understood that, when the loading direction is close to the molecular direction (i.e., in case of a small orientation angle), relatively hard covalent bond inside molecule (for stretch or bending) can effectively resist to the loading. In this study, it is suggested that the microscopic spiral structure of TC fibers/fibrils plays an essential and effective role to provide a good performance needed for a strong and tough material.

Keywords: Molecular dynamics(MD), Collagen, Natural polymers(proteins), Spiral, Strength, Mechanical properties, Structural mechanics, Computational mechanics

References

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