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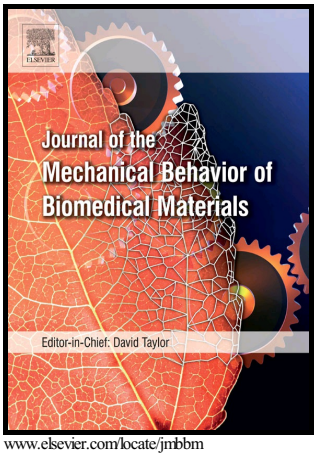

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Steered molecular dynamics characterization of the elastic modulus and deformation mechanisms of single natural tropocollagen molecules

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Abstract

Collagen is a common structural protein, providing mechanical integrity for various vertebrate connective tissues such as cartilage and bone. The mechanical behaviours of these tissues under physical stimulations are controlled by the hierarchical structure of collagen and its interactions with other extracellular matrix molecules. However, the mechanical properties and deformation mechanisms of natural collagen under physiological loading rates at the molecular level are not fully understood. In this study, comprehensive steered molecular dynamics (SMD) simulations were performed on the 2nd intact overlap region (d2ol) and the 2nd intact D-period (d2olgp) of an in-situ characterized collagen molecule, under a large range of strain rates (6.5×10^{6}%.s^{-1} to 1.3×10^{12}%.s^{-1}). The results show that, depending on the applied strain rates, tropocollagen molecules unfold in different ways. Particularly, at high and intermediate strain rates, the number of inter-chain hydrogen bonds decreases rapidly even at small deformations, leading to a dramatic increase in the force. This results in an increase in the estimated Young's modulus of collagen triple helices as the deformation rate goes up, which, together with the nonlinear mechanical behaviour, explains the broad range of the Young's modulus for collagen model peptides reported in earlier SMD studies. Atomistic-level analyses indicate that the elastic modulus of single tropocollagen molecules decreases as the strain rate becomes smaller.