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Mechanical Response Study of Collagen by means of Molecular Simulation PIETER J. IN 'T VELD, Sandia National Laboratories, MARK J. STEVENS — We developed a coarse-grained model to study mechanical behavior of collagen fibrils as a function of their degree of cross-linking. A collagen molecule is represented by Lennard-Jones beads, which intra-molecularly are connected through harmonic springs on both bond length and angle. In this model each bead represents a helical turn in a collagen molecule. Triple-helical collagen molecules, which are 300 nm long, are packed within fibrils in a staggered fashion with an axial spacing of 67 nm in the absence of a load on the tendon. We treat the outer layer or shell different from the core by assuming the shell has the maximum amount of available cross-links. The core has a variable amount of cross-links by allowing cross-link formation and breakage depending on a reaction-type criterion. We study the stress-strain behavior of a single fibril through tensile deformation along the principal axis and a three-point bend perpendicular to the principal axis.

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