Constructing a Coarse-Grained Model for Cross-Linked Collagen Fibrils

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Collagen fibrils are microscopic molecular ropes that are structural components in many animal tissues. We present an equilibrium coarse-grained model for the structural and mechanical properties of these cross-linked fibrils. We model enzymatic cross-links as anisotropic Gaussian chains, which allows us to approximate their free-energy contributions. We add additional free energy terms for the Frank elastic energy due to the orientation of collagen molecules within the fibril, for the surface tension, and phase-field crystal terms which account for the D-band density modulations observed along the length of collagen fibrils. We computationally minimize the sum of these free-energy terms given an imposed strain field acting on the fibril to obtain equilibrium structures. Using this framework we investigate the effect of strain on various important structural and mechanical properties of the fibril, such as the molecular director field, characteristics of the D-band, and the stress-strain curve.