Silk fiber mechanics from models at different length scales

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Silk is one of the most resilient fibers in nature. Consisting of an amorphous matrix cross-linked by beta-sheet rich crystalline units, silk is a hierarchically organized material the molecular details of which remain largely unknown. In order to decipher the structural determinants of its mechanical properties, we model silk at different length scales by combining molecular dynamics simulations, force distribution analysis, and finite element methods. We predict the distinct mechanics of anti-parallel versus parallel silk crystals as force-bearing cross-links [1], and the impact of chain entanglement and crystallinity on fiber mechanics [2]. Our predictions can serve as a guide for the design of artificial silk protein analogues.

[1] Xiao S, Stacklies W, Cetinkaya M, Markert B, Gräter F., Mechanical response of silk crystalline units from force-distribution analysis.(2009) Biophys J.,96(10):3997-4005.
[2] Cetinkaya M., Xiao S., Graeter F., et al, in submission.