Geometric Frustration Selects Morphology in Chiral Filament Bundles

DOUGLAS HALL, ISAAC BRUSS, UMass Amherst, JUSTIN BARONE, Virginia Tech, GREGORY GRASON, UMass Amherst — Assemblies of twisted filaments appear in a range of biological contexts, from extracellular filament bundles to amyloid fibrils. Owing to numerous distinctions in molecular structures and interactions underlying these diverse assemblies, a framework to predict and classify the basic mechanisms of structure formation in twisted filament assemblies is still lacking. In this study, we model how the size and shape of self-assembled fibers are controlled by competition between the elastic costs of inter-filament frustration, bending deformation of filaments and bundle surface energy. Exploiting a geometric mapping between inter-filament packing in twisted bundles and packing on positively-curved 2D surfaces, we show that the anisotropy of the bundle cross-section is determined by a single parameter describing the competition between elastic and bending costs. We compare the continuum model’s predictions for stability of cylindrical and tape-like twisted morphologies to numerical simulations of cohesive filament bundles and observations of micron-scale amyloid fibers assembled from hydrolyzed protein fragments.

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