Geometrical Frustration and Lattice Defects in Twisted, Two-Dimensionally Ordered Filament Bundles

GREGORY GRASON, Department of Polymer Science and Engineering, University of Massachusetts, Amherst — We study a continuum-elastic description of filament assemblies, bundles or fibrils, that are two-dimensionally organized in cross-section while simultaneously adopting a globally twisted structure. In this model, twisting may occur in response to external forces or as a consequence of the intrinsic interfilament torques acting between chiral macromolecules, like F-actin and collagen, ubiquitous in biological systems. We show that the geometrical, non-linear couplings between tilt and in-plane strain required by the elastic description of ordered filament arrays frustrate the lattice packing of filaments in precisely the same way that out-of-plane deflection frustrates the formation of two-dimensional crystals on curve surfaces. Hence, the elastic cost of forming a twisted bundle corresponds directly with the stretching cost of arranging crystal on a sphere of an appropriate radius. Based on this mapping we demonstrate that above a critical size, a twisted bundle is unstable to the incorporation of a finite number of line disclinations, that partially screen the twisted-induced stresses. We present results on the complex spectrum of groundstate bundle packings that result from the consideration of stress-localizing, lattice defects and discuss the implications of the defect-riddled groundstates for the mechanics and thermodynamics of self-assembled molecular filaments.