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Simulating Topological Defects in Twisted Fiber Bundles[1] ISAAC R. BRUSS, GREGORY M. GRASON, Department of Polymer Science and Engineering, University of Massachusetts, Amherst — Twisted bundles are a common motif found in naturally occurring structures of self-assembled fibers, such as collagen and fibrin. By understanding the general principles governing such organizations, new synthetic materials–from the nano to the macroscale–may also be realized. Recently, continuum elasticity theory has been applied to describe generic twisted fiber bundles. This has revealed a relation between a bundle's twist and the presence of topological defects in the cross-sectional packing of the fibers. Here we employ numerical simulations to examine this interdependence. We model a bundle's cross-section as beads confined to a plane. The interactions between beads is governed by a modified Lennard-Jones potential that accounts for the effects of twist. We observe configurations that range from perfect hexagonal packing for cases of no twist, to defect populated structures above a critical amount of twist. For small bundles of less than $\sim$100 beads, there exists a discrete spectrum of energy ground states corresponding to integer numbers of five-fold disclinations. For larger bundles, we hope to uncover what types of defect arrangements effectively screen the stresses caused by twist, and compare these to current predictions of the internal organization of collagen fibrils.

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