Self-Limited Self-Assembly of Chiral Subunits

Yasheng Yang, Robert Meyer, Michael Hagan Brandeis MRSEC (DMR 0820492)

A simple computational model demonstrates the assembly of self-limited filamentous bundles. The images are taken from dynamic Monte Carlo simulations in which chiral subunits spontaneously assemble under different interaction strengths and degrees of (a) Moderate interactions and chirality. moderate chirality reproducibly lead to a selflimited bundle with three layers of subunits, while stronger chirality (b) results in a selflimited two-layer bundle. (c) With strong interactions, frustration is relieved by defects, which enable the formation of branched networks and irregular bundles. These complex structures, which spontaneously emerge from the dynamical simulations, could not have been predicted with geometrical equilibrium arguments.

