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Equilibrium Fold Thickness in Polymer Crystals BUCKLEY CRIST, Northwestern University, HERVE MARAND, Virginia Tech — It has been accepted for nearly four decades that the limited thickness of folded chain polymer crystals results from secondary nucleation barriers. In recent years, however, simulations of polymer crystallization indicate that the observed crystal thickness is a consequence of free energy minimization, not kinetic pathways. An analysis in terms of classical (homogeneous) nucleation theory indeed gives a column-like equilibrium crystal shape (thickness/width > 1) that results from anisotropic surface energies. All dimensions increase commensurately as the crystal grows, with the equilibrium thickness approaching the extended chain length when an unlimited number of chains are available to crystallize. Beyond a certain point in the growth process, however, one expects nucleation barriers to favor less thick crystals that have non-equilibrium, plate-like shapes. For simulations done with a limited number of chains the equilibrium crystal thickness is observed because the crystal is small. But one should not conclude that equilibrium dictates the dimensions at later stages of crystal growth.

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