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Block copolymers in cylindrical confinement: role of thermal fluctuations and confinement parameters in structure formation KIRILL TITIEVSKY, Massachusetts Institute of Technology — Phase segregated block copolymer morphology and dimensions were studied using explicit simulations of interacting bead-spring chains at physically realistic densities. In particular, The distribution of characteristic morphologies and structure dimensions for a given fiber diameter are characterized. Key novel aspects of this work inlude sampling of thermal fluctuations in full three dimension, rather than finding minimum energy surfaces and extensive comparison to experimental data on electrospun block copolymer–polymer fibers. Two methodological innovations are also introduced. First, an unprecedentedly precise estimate of Flory χ parameters for the model allows a quantitative comparison to field theoretic models. Second, a novel reflective boundary model allows common boundary artifacts in total density to be effectively eliminated, even for fibers with of dimensions comparable to single chains.

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