

Process-Directed Self-Assembly of Block Copolymers

Marcus Mueller^{C, S} and De-Wen Sun

Institute for Theoretical Physics, University of Goettingen, Goettingen, Lower Saxony, Germany
mmueller@theorie.physik.uni-goettingen.de

Process-directed self-assembly of block copolymers refers to rapid thermodynamic processes that reproducibly direct the kinetics of structure formation from a starting, unstable state into a selected, metastable mesostructure. We investigate the kinetics of self-assembly of linear block copolymers after different rapid changes of thermodynamic control parameters (e.g., photochemical transformations [1], stretching or mechanical deformation [2], or pressure changes [3]). These thermodynamic processes convert an initial, equilibrium mesophase of the copolymer material into a well-defined but unstable, starting state. The spontaneous structure formation that ensues from this unstable state becomes trapped in a metastable mesostructure, and we systematically explore, which metastable mesostructures can be fabricated by varying the physical properties of the copolymers in the starting and final state and a step-shear deformation. In addition to the equilibrium mesophases of linear AB diblock copolymers, this diagram of process-accessible states [1] includes multiple, novel, metastable periodic mesostructures; inter alia, Schoen's F-RD periodic minimal surface. Generally, we observe that the final, metastable mesostructure of the copolymer possesses the same symmetry as the initial, equilibrium mesophase of the copolymer. Strategies and challenges for studying process-directed self-assembly by particle-based simulations and self-consistent field theory are discussed and the role of non-equilibrium chain conformations and the diffusive dynamics is highlighted.

References:

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- [3] Directing the self-assembly of block copolymers into a metastable complex network phase via a deep and rapid quench, M. Müller and D.W. Sun, Phys. Rev. Lett. 111, 267801 (2013)