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Stability of sphere-forming phases in diblock copolymers: Assessment of lattice-partition theories AKASH ARORA, FRANK S. BATES, KEVIN D. DORFMAN, Department of Chemical Engineering and Materials Science, University of Minnesota - Twin Cities, Minnesota, USA — The recent experimental discovery of a Frank-Kasper σ phase in block copolymers has significantly altered our understanding of the sphere-forming region of the phase diagram. The σ phase possesses a large tetragonal unit cell containing 30 particles of different shapes and sizes, arranged in three different coordination environments. Although self-consistent field theory (SCFT) calculations have successfully identified the importance of conformational asymmetry on the relative stability of body-centered cubic (BCC) and the σ phase, the dependence of stability of the σ phase to its space-filling or lattice-partition principles remains an open question. In this study, we examine different geometrical theories in literature that attempt to predict the stable phase directly from the shapes and sizes of different Wigner-Seitz cells comprising the lattice. Specifically, we compare the predictions from these theories for four phases, fcc, bcc, σ , and A15 in diblock copolymers, to the results of SCFT calculations over a wide range of the sphere-forming region of the phase diagram. Our results bring to the fore both the successes and failures of purely geometric theories to predict the relative stability of these phases in diblock copolymers.

Akash

Department of Chemical Engineering and Materials Science, University of Minnesota - Twin Cities, Minnesota,

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