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Block Copolymer Droplets: The Interplay of Surface Energy and Ordering SU-MI HUR, ABELARDO RAMIREZ-HERNANDEZ, Institute for Molecular Engineering, University of Chicago, M. SERDAR ONSES, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, PAUL NEALEY, Institute for Molecular Engineering, University of Chicago, JOHN A. ROGERS, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, JUAN J. DE PABLO, Institute for Molecular Engineering, University of Chicago — Monte Carlo simulations of a coarse-grained model are used to explore the morphology of block copolymer droplets on a flat substrate. The characteristic size of the droplets is on the order of several natural periods of the block copolymer morphology in the bulk. In this regime, the equilibrium morphologies inside the droplets and their shapes arise from a subtle interplay of interfacial and bulk contributions to the free energy. While a simple fluid droplet on a flat substrate exhibits a spherical cap shape, nanostructured block copolymer droplets are found to adopt unusual shapes, such as conical-shaped droplets with a terraced surface or pancake-shaped droplets. Our simulation results predict non-circular arrangements, with perpendicular domains, when the block copolymer is deposited on a neutral substrate regardless of size. However, when a preferential substrate is used, a dependence on droplet size is observed: block copolymers form a pancake-shaped droplet with a ring of perpendicular domains along the perimeter for large droplets, while they exhibit perpendicular domains when the droplet is small. These results are in very good agreement with experiments.

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