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Shear-induced sphere-to-cylinder transition in thin films of diblock copolymers and the role of wetting layers ALEXANDROS CHREMOS, RICHARD REGISTER, Princeton University, PAUL CHAIKIN, New York University, ATHANASSIOS PANAGIOTOPOULOS, Princeton Unversity — The shear-induced sphere-to-cylinder transition in diblock copolymer thin films has been studied using large-scale coarse- grained Langevin dynamics simulations. At zero-shear conditions and below the order-disorder transition temperature the thin film forms a monolayer or bilayer of spheres given the thickness of the film. Mimicking the experimental setup the minority block has an affinity to be adsorbed on the confining surfaces forming brushes which interpenetrate the rest of the film. Once a shear field is applied and above a critical shear rate, the spheres elongate and merge with their neighbors to form cylinders. We find that the mechanism with which the spheres merge is closely related with the stretching of individual diblock chains. In particular, we find that in monolayer thin films it is more difficult to achieve the sphere-to-cylinder transition, which is also an experimental observation, because the brushes restrict the stretching of diblock chains. The simulations were performed with the use of Graphical Processing Units allowing large-scale simulations with long polymer chains to studied.

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