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Shear induced alignment in thin bilayer films: a simulation study JOERG ROTTLER, Dept. of Physics and Astronomy, University of British Columbia, 6224 Agricultural Road, Vancouver, BC V6T 1Z1, DAVID J. SROLOVITZ, Dept. of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ 08544, PAUL CHAIKIN, Physics Dept., New York University, 4 Washingon Place, New York, NY 10003 — Motivated by recent experimental progress, we study ordering mechanisms in confined bilayer systems under shear via Brownian dynamics simulations. In sphere-forming thin block copolymer films, spherical nanodomains arrange in grains of local hexagonal symmetry, but random orientation. If the film has precisely the bilayer thickness, the application of simple shear leads to global, macroscopic alignment in a triangular lattice (D. Angelescu et al., Adv. Mat. 17, 1878 (2005)). By representing each nanodomain a as purely repulsive sphere on a coarse-grained level (therefore making the model also applicable to colloidal assemblies), our simulations reveal that the long range order can develop through the shear induced motion of grain boundaries rather than global melting and recrystallization. The time dependence of this process may be described by Avrami growth laws. In order to gain further insight into the microscopic mechanism of shear induced ordering, we study the motion of single domain walls in simplified geometries and determine the dependence of the grain boundary migration velocity on geometry, shearing conditions and the resulting local stress gradients.

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