Defect Motion and Annihilation in Block Copolymer Thin Films

Marcus Müller [C, S] and Weihua Li
Institute for Theoretical Physics, Georg-August University, Göttingen, Germany
mmueller@theorie.physik.uni-goettingen.de

Using self-consistent field theory and computer simulation of a soft, coarse-grained particle model we study defect motion and annihilation in thin films of lamella-forming block copolymers on neutral and chemically patterned substrates. By virtue of the strain-field mediated interactions, dislocation defects with opposite orientation move towards each other. This motion depends both on the thermodynamic, strain-field mediated driving force and the single-chain dynamics that is required to alter the morphology and reduce the distance between the defect cores. This interplay results in a qualitative dependence of the time evolution on the topology of the defect morphology. Upon collision of the defects, they either spontaneously annihilate or form a metastable, tight defect pair. In the latter case, a free-energy barrier has to be overcome to finally produce a defect-free structure. Computing the minimum free-energy path within self-consistent field theory we investigate the dependence of the free-energy barriers of defect motion and annihilation on incompatibility, strength of the chemical surface pattern, and defect morphology.