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Kinetic Aspects of Defect Annihilation in Block Copolymer Thin Films on Patterned Substrates. SU-MI HUR, University of Chicago, PAULINA RINCON-DELGADILLO, IMEC, VIKRAM THAPAR, Cornell University, ABELARDO RAMÍREZ-HERNÁNDEZ, Argonne National Lab., GURDAMAN KHAIRA, PAUL NEALEY, University of Chicago, MARCUS MÜLLER, Institut fur Theoretische Physik, JUAN DE PABLO, University of Chicago — Although there has been significant progress on understanding various aspects of directed self-assembly of block copolymers at equilibrium, important challenges remain regarding the development of materials and processes leading to a perfect, defect-free assembly. We present minimum free-energy pathway calculations for annihilation of dislocation defects in block copolymer thin films using the string method combined with a Theoretically Informed Coarse-Grained (TICG) simulation approach. Our results demonstrate the importance of kinetics in the elimination of defects, where an extraordinarily large thermodynamic driving force is not necessarily sufficient for defect removal. The kinetic path follows fully three-dimensional morphological changes; the corresponding transition states often consist of a very slight connection between an edge dislocation and the neighboring domain. Investigation of the transition states provides useful insights into the possible rate-determining mechanisms for defect motion. We also explore the dependency of the kinetic-energy barriers on the defect type and position, and on processing conditions such as the type of chemical pattern or the strength of the segregation force between the blocks.

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