

Reorientation of microdomains in cylinder forming diblock copolymer thin films during solvent vapor annealing: simulations with dissipative particle dynamics

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Solvent vapor annealing (SVA) is an efficient technique to refine and control the structure of ordered block copolymer films, promising as functional templates for nanolithography and membrane preparation. SVA was simulated in the case of intermediate A/B block segregation and fast solvent evaporation. Under these conditions, the domain orientation is controlled by the solvent selectivity. If the solvent preferentially dissolves the short blocks, lying cylinders in thermodynamic equilibrium appear. In contrast, solvents selective for the long blocks reorient the cylindrical domains along the solvent concentration gradient, i.e. vertically. This may be explained by the Gibbs-Marangoni effect and by the interplay of adsorption of the short and the long blocks at the two film interfaces. Longer film drying, attained after strong initial film swelling in a moderately good solvent, produces the most ordered films. The mechanism of the film evolution is discussed in detail.

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