
Concentrated dispersions and melts from micellar solution: computer simulation by dissipative particle dynamics

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Abstract

It is well-known that the process of microphase segregation, that occurs in the melts of thermodynamically incompatible block-copolymers, leads to the formation of ordered structures with different morphologies (spherical and cylindrical domains of one phase into another, lamellar structures, gyroid structures, etc). However, the formation of a segregated film with well-defined order is a complicated problem from the viewpoint of technical implementation owing to a number of labor-intensive procedures, such as selection of common solvent, regime of solvent evaporation and film annealing. To investigate the production of nano- and micro-structured films, the approach, which is based on film formation by solvent evaporation may be proposed. In this research we study the films formed by block-copolymer micelles (core-shell particles) by means of DPD (dissipative particle dynamics) simulation technique. We test the melt stability and compare melt structure with previously obtained results for preliminary formed macromolecular objects.

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