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A new field-theoretic simulation method for compressible systems containing block copolymers JUNHAN CHO, Dankook University — A new field-theoretic simulation method based on a compressible random-phase approximation (RPA) theory has been suggested to understand the self-assembly behavior and its pressure responses of compressible systems containing block copolymers. Finite compressibility is incorporated in the free energy functional for the dissipative dynamics through effective RPA interactions that account for the excluded volume and the attractive nonbonded interactions. It was shown for A-b-B copolymer melts in unconfined or confined geometry that basic equation-of-state parameters completely characterizing given block components readily yield stable and metastable morphologies without any presumed symmetry over a wide range of temperature-pressure-composition space. It was demonstrated that the simulation tool is capable of predicting in a unified way the self-assembly behavior not only exhibiting nanoscale ordering either upon cooling or reversely upon heating, but also revealing barotropicity and baroplasticity. The simulation of the self-assembly behavior of multiblock copolymers with diverse molecular architectures and also of block copolymers in a solvent covering from complex patterns to micellar structures was also discussed.

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