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Molecular dynamics study on microstructures of diblock copolymer melts with soft potential and potential recovery[1] SEULWOO KIM, JI HO RYU, Seoul Natl Univ, HAN SOL WEE, Purdue University, WON BO LEE, Seoul Natl Univ — The method for obtaining various self-assembled microstructures with block copolymers, was investigated using molecular dynamics (MD) simulation. However, it requires expensive computational cost time to prepare initial configurations of various self-assembled structures because of topological constraints. Furthermore, manual preparation often becomes a complicated and time-consuming procedure even for the simplest structures, a lamellar phase, not to mention more complicate phases, such as a gyroid phase. The difficulty may be overcome by introducing a soft potential, which allows the system to reach a self-assembled state quickly (within $3\tau_d$). Once a self-assembled microstructure is obtained, the normal potential, for instance, Weeks-Chandler-Andersen (WCA) potential, is restored and equilibration runs are performed to calculate various properties of the microstructures. With our approach, various equilibrated phase structuresincluding S (spherical), H (hexagonal), G (gyroid), and L (lamellar) phasesare obtained. To verify our method, static and dynamic properties of the lamellar phase are examined with previous results.

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