Molecular dynamics simulation for several block copolymer Self-Assembly system

남정용, 이원보†
서울대학교
(wonbo.lee@gmail.com†)

In this study, the Self-assembly behavior of several block copolymer could be developed by Molecular Dynamics(MD) simulation. To put Molecular Dynamics briefly, it uses Newtonian equation of motion. The force consists of bond force, angle force, dihedral force, pair force, etc. After calculating force, Molecular dynamics needs initial momentum and position. With this, we can compute updated momentum and position via Newtonian equation of motion. By using molecular dynamics, the trajectory of block copolymer self-assembly can be obtained and the topology of equilibrium state of self-assembly can be acquired. The Topology of several block copolymer shifts when the portion of block copolymer changes or when the force between monomers change. Those contents will be described in this study.