Fast field theoretic simulation of block copolymers with the mode Monte Carlo method

YONGJOO KIM, ADAM HANNON, CAROLINE ROSS, ALFREDO ALEXANDER-KATZ, MIT — We explore the self assembly of block copolymers by using a field theoretic simulation method. Former studies on field theoretic simulation methods update the fields by Langevin-like dynamics which is a local update of the fields in real space. Our simulation method updates the mode structure (k-space) of the fields and transfers them to real space. By using a Monte Carlo scheme for updating fields, we decrease simulation time by nearly an order of magnitude. We also consider new self-learning searching strategies using this method. We tested our algorithm by simulating the phase diagram for thin films of diblock copolymers in select graphoepitaxial templates and by simulating the self-assembly of nanoparticles and block copolymers.