Numerical Methods of Self-Consistent Field Theory

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The phase diagram of the equilibrium states and the stability of the possible microstructures are both important for polymer scientists. The phase behavior of a copolymer system could be studied through self-consistent field theory (SCFT). Though the numerical methods in both Fourier space and real space have been successfully applied to calculate the structure of the phases, both have advantages and disadvantages. The new numerical implementations of SCFT included iteration and initial values are developed to investigate the phase behavior of the diblock copolymer system. Though the method is based on the Fourier expansion of order parameter, a priori symmetric information is not required, and more significantly, the period structure can be adjusted automatically during the iteration as well. The method enables us to calculate the phase diagram, discover new meta-stable phases, verify the epitaxial relation in the phase transition process.

We will also introduce a numerical method to study the nucleation in copolymer melts. Nucleation is the decay of a metastable state via the thermally activated formation and subsequent growth of droplets of the equilibrium phase. We will consider the nucleation in diblock copolymer melts, whose equilibrium phases are well understood. We apply a new numerical method, called the string method, to compute the minimum energy path (MEP). Then from the MEP, we find the size and shape of the critical droplet and the free-energy barrier to nucleation.