Numerical Methods for Ordered Patterns in Polymeric Systems

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Discovering ordered structures is an eternal topic in science. Theoretical approaches to investigating the emergence and stability of an ordered phase often involve minimizing an appropriate free energy functional of the system, and comparing the free energies of different candidate structures. The main features of the energy functionals include nonlinearity, and multi-solutions. Analytically finding all solutions of these models is beyond today's technology. An alternative approach is turning to numerical investigation. In this talk, we focus on the development of numerical methods for the periodic and quasiperiodic structures in polymeric systems. A systematical numerical framework has been proposed to explore the ordered structures, including the strategies of screening the initial values, targeted discretization methods, and the approach of adaptively optimizing computational box. We apply the numerical methods to the self-consistent-field theory, a widely used theory in polymeric systems. A large number of ordered structures have been discovered in related block copolymer systems which are consistent with the experimental results. Furthermore, several soft quasicrystals have been explored using the recently developed projection method based on the Landau-type models.