Simulation of complex fluids with multiple intrinsic lengths

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Ginzburg-Landau models are widely used in mesoscopic simulations of condensed matter. Numerical minimization of a free energy functional is often useful in finding the equilibrium structures in the ordered phases. However, some highly complex structures possess multiple intrinsic lengthscales, which cause a difficulty in the simulation. To reproduce the correct equilibrium structure, the size of the simulation box must be commensurate with the intrinsic lengthscales, which are not known beforehand in general and/or are not commensurate with each other. In such cases, the choice of the boundary condition is a crucial problem. A conventional boundary condition (such as the periodic and Neumann) will not lead to true equilibrium patterns.

In this study, we introduce new boundary conditions that circumvent this difficulty, using a binary mixture of diblock copolymer melts and a chiral liquid crystal system as examples. The former in the lamellar-lamellar coexistence has two characteristic lengths, i.e., the lamellar thicknesses in the two phases. The latter in the twist grain boundary (TGB) phase has three, which are the layer thickness, the distance between grain boundaries, and the distance between dislocations in a grain boundary.

For the lamellar-lamellar coexistence in copolymers, we introduced the "local equilibrium boundary condition" [1]. In this scheme, the time-evolution at any bulk site a obeys the standard diffusive equation,

$$\frac{\partial \psi_a^{(i)}}{\partial t} = \nabla^2 \frac{\delta F}{\delta \psi_a^{(i)}}, \tag{1}$$

where $\psi^{(i)}$'s are linear combinations of the segment densities of the four types of blocks and $F = F[\{\psi^i\}]$ is the appropriate free energy. For any boundary site b, we assume the evolution equation

$$\frac{\partial \psi_b^{(i)}}{\partial t} = -\frac{\partial}{\partial \psi_b^{(i)}} \sum_a \left(\nabla^2 \frac{\delta F}{\delta \psi_a^{(i)}} \right)^2, \tag{2}$$

where the summation runs over the bulk sites in the neighbor of b. With this equation, the order parameter at the boundary site evolves so that the neighbor bulk sites approach local equilibrium. This equation is heuristic, but works well when the initial condition is close enough to the equilibrium state (see Fig.1).

The TGB phase of chiral liquid crystals is achieved by the balance between the smectic layering order and the chirality. The chirality requires careful treatment of the boundary condition in the direction along the helical axis, because the twisting free energy appears only as a boundary term in the standard time dependent Ginzburg-Landau scheme. On the other hand, for the direction perpendicular to the helical axis, we use the boundary condition that automatically adjusts the system size to the smectic slab thickness and the distance between dislocations.

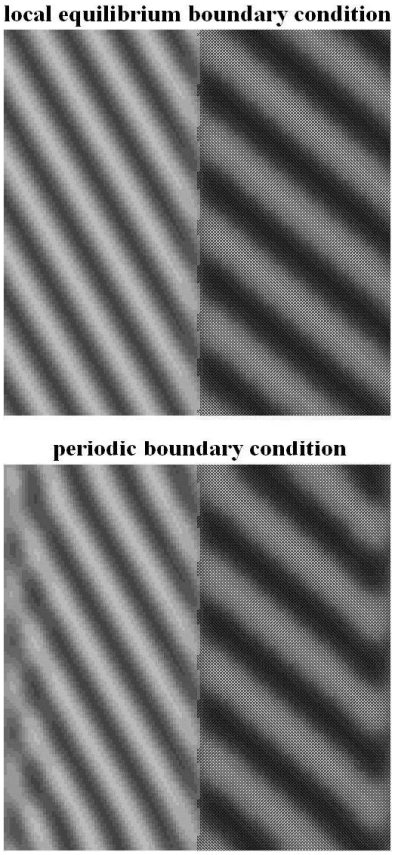

Figure 1: Lamellar-lamellar coexistence patterns obtained with the periodic and the new boundary conditions. With the periodic boundary condition, the lamellar is deformed near the system boundary.

References

[1] H. Ogawa, and N. Uchida, Phys. Rev. E submitted.