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Epitaxial Transition from Gyroid to Cylinder in a Diblock Copolymer Melt

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1 Introduction

In the past, the self-organized microdomain structures of diblock copolymers have been the target of extensive studies both experimentally and theoretically. Among various microdomain structures, the bicontinuous double gyroid (G) structure has attracted a great interest because of its complex but highly symmetric structure. We simulated an order-order transition from a G structure to a hexagonally packed cylinder (C) structure induced by an external flow in [111] direction of the G unit cell using real-space dynamical self-consistent field technique. In order to simulate the structural change correctly, we introduce a system size optimization (SSO) technique by which emergence of artificial intermediate structures are suppressed.

2 SSO method

To obtain equilibrium states of the periodic microdomain structures of G and C, we regard the side length of the simulation box \( L_i \) \((i = x, y, z)\) as a dynamical variable whose dynamics is described by the following fictitious equation of motion

\[
\frac{\partial L_i}{\partial t} = -\zeta_i \frac{\partial (F/V)}{\partial L_i},
\]

where \( F \) is the free energy of the system and \( V \) is the volume of the system. The coefficient \( \zeta_i \) is a damping coefficient that ensures numerical stability. The total energy of the system is given by

\[
E = \frac{1}{2} \sum_i \left( K_{ij} \frac{\delta L_i}{\delta L_j} + \phi_i \right) \delta L_i \delta L_j
\]

where \( K_{ij} \) is the elastic constant and \( \phi_i \) is the chemical potential of species \( i \).

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where \( \frac{f}{\nu} \) is the free energy density and \( \zeta_i \) is a positive coefficient. We checked the validity of this equation and found that the most appropriate value of the \( \zeta_i \) is 0.05 for the C phase \( (\chi N = 15, \text{block ratio } f = 0.35) \).

### 3 Results and Discussion

The temporal change of the G periodic cell under a shear flow to the [111] direction and a sudden temperature change from \( \chi N = 20 \) to \( \chi N = 15 \) is shown in Fig. 1. The G structure is deformed by the shear flow as shown in Figs. 1(a) and 1(b). A small domain of cylinders is generated in Fig. 1(c), which is indicated by an open arrow. The transition from the G structure to the C structure takes place at the lower grain boundary of this C domain as shown in Figs. 1(d)-(f). This transition reproduces a nucleation of the C domains. The generated C domains grow epitaxially, where the \{220\} planes of the G structure coincide with the \{10\} planes of the C structure (so called epitaxial growth) as Fig. 2, while the theoretical studies in reciprocal space and the experimental studies suggest \{211\} to \{10\} transition [1].

![Fig. 1 Time evolution of the domain in the OOT G \( \rightarrow \) C.](image)

![Fig. 2 Projection of the G unit cell structure observed from the [111] direction. The circles indicate the positions of the cylindrical domains in the epitaxial transition (a) G \{211\} \( \rightarrow \) C\{10\} and (b) G \{211\} \( \rightarrow \) C\{10\}, respectively.](image)

### References

[1] T. Honda and T. Kawakatsu, Macromolecules. 39 (2006), 2340.