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Rhombohedral structure observed in the computer simulations of block-copolymer melts

A. Saeki (1), F. Yonezawa (2)
(1) Comp. Sci & Eng. Dept., Nagoya Univ., Japan
(2) Dep. Phys., Keio Univ., Japan

Diblock copolymer melts show various ordered structures, such as cylinders(C), lamellae(L), and a gyroid structure(G), depending on the temperature and the constitution ratio of two different homopolymers, each consisting of A or B monomers alone. A gyroid structure has a three-dimensional bicontinuous network with \( I_{h3d} \) symmetry and negative Gauss curvature.

We carry out computer simulations of diblock copolymer melts, from which we discover a gyroid-like structure between the cylinder phase and the lamellar phase. Our computer simulation of diblock copolymer melts is based on the scheme, the extended Cahn-Hilliard equations which enables systems to reach to the most stable state rather easily.

\[
\frac{\partial}{\partial t} \phi(r) = \Delta \left( -A\psi + \psi^3 - D\Delta \psi \right) - B\psi, \quad \frac{\partial}{\partial t} \psi(r) = \phi(r),
\]

in which we have introduced the momentum of the field \( \phi \) as a new term in addition to the ordinary terms in the CH equation.

The results of simulations are shown in Figs. 1-3 in which the illustrations of the surface of a constant \( \phi \) value are presented from three different angles.

![Fig.1](Fig1.png) ![Fig.2](Fig2.png) ![Fig.3](Fig3.png) ![Fig.4](Fig4.png)

The unit cell of this gyroid-like structure is rhombohedral as shown in Fig.4. There are two ways to define the unit cell of rhombohedral-type, i.e., a way in which the a- and b-axis are respectively orthogonal to c-axis, and the other way in which the each length of a- and b- and c-axis is taken to be the same. Here the former way is adopted. In Fig.4, both a- and b-axis are orthogonal to c-axis. The angle between the a-axis and the b-axis is \( \pi/3 \). The length in the a-direction of a unit cell is the same as that in the b-direction. The ratio of the length in the a-direction (or b-direction) to the length in the c-direction is \( 1/2.1 \); in other words, \( a : c = 1 : 2.1 \), which is found from our computer simulations. From analyzing Fig.4, we can decide the space group symmetry of this gyroid-like structure to belong to \( R3c \), where the index \( R \) represents rhombohedral, and \( 3 \) represents a three-fold rotoinversion symmetry, while \( c \) means a glide reflection symmetry as to the c-axis.

From the recent studies of scattering experiments by Imai et al., it has been shown that there exists a structure with \( R3c \) symmetry which appears in the process of L-to-G transition in the nonionic surfactant/water system.