<table>
<thead>
<tr>
<th>Title</th>
<th>P16 Rhombohedral structure observed in the computer simulations of block-copolymer melts</th>
</tr>
</thead>
<tbody>
<tr>
<td>Author(s)</td>
<td>Saeki, A.; Yonezawa, F.</td>
</tr>
<tr>
<td>Citation</td>
<td>物性研究 (2002), 79(2): 250-250</td>
</tr>
<tr>
<td>Issue Date</td>
<td>2002-11-20</td>
</tr>
<tr>
<td>URL</td>
<td><a href="http://hdl.handle.net/2433/97327">http://hdl.handle.net/2433/97327</a></td>
</tr>
<tr>
<td>Type</td>
<td>Departmental Bulletin Paper</td>
</tr>
<tr>
<td>Textversion</td>
<td>publisher</td>
</tr>
</tbody>
</table>

Kyoto University
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 $I_{a3d}$ 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.

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

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 $\psi$ value are presented from three different angles.

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 $R\bar{3}c$, where the index $R$ represents rhombohedral, and $\bar{3}$ 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 $R\bar{3}c$ symmetry which appears in the process of L-to-G transition in the nonionic surfactant/water system.