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Micro Structure Analysis of Liquid Crystal Using X-ray Anomalous Dispersion Effect

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Introduction

It may be an interesting problem to determine the position of molecules doped into substances, giving us the information on the interaction between them. For such a purpose, the X-ray anomalous dispersion technique could be utilized. We can distinguish the dopant and host molecules by making an X-ray measurement around the absorption edge of the dopant with changing the energy of the incident beam. In this report we have made an attempt to determine the position of Cu molecules doped into a smectic liquid crystal with layered structure.

Experimental

We used poly(oxyethylene) cholesterol (POE) exhibiting the smectic A phase and copper(II) 4-heptylcyclohexylcarboxylate (CuHCC). Measurements were made in a 2% CuHCC-doped POE. Since the layer spacing is about 71 Å at room temperature, we used BL10C for small-angle X-ray scattering (SAXS) in Photon Factory of KEK. SAXS intensities were measured as a function of the wavelength around the Cu-*K* absorption edge from 1.3762 to 1.3855 Å. The energy of the incident X-ray was tuned with a double monochromator of Si. The scattered X-ray was detected with a one-dimensional detector and the intensity was accumulated for 150 sec at each step.

Results and discussion

The smectic liquid crystal is a one-dimensional crystal and so we can observe only the reflections with 00*l*. In our experiment, 001 and 002 were observed. Figure 1 shows the wavelength dependence of the integrated intensity of the 001 reflection. It is clearly seen that the integrated intensity peaks at the absorption edge. This result indicates that the dopant molecules are located between layers, as shown in the following consideration.

For a simple model that Cu atoms are dispersed in the smectic liquid crystal without correlation, the scattering intensity is given as

$$I_k = \rho_k^2 + 2f'\rho_k n_k + |f|^2 (n_0 + n_k^2), \qquad (1)$$

where ρ_κ and n_κ are, respectively, the Fourier transforms of the electron density of the smectic liquid crystal and the averaged number density of the Cu atoms, and f is the atomic form factor of Cu atom. Note that in the smectic liquid crystal we can take ρ_κ and n_κ as real numbers.

For a small amount of dopant, the third term of r.h.s. in eq. (1) can be omitted. The first term is the contribution from the host smectic liquid crystal and the second term, more importantly, expresses the spatial correlation between the host and the dopant. Around the absorption edge, the real part, f', decreases as shown in Fig. 1, whereas the intensity increases at this point. From these results and the second term of eq. (1), $\rho_\kappa n_\kappa$(κ is for the 001 reflection) should be negative. This means the phase difference between the fundamental density waves of the host and the dopant is 180 degrees and therefore the dopant molecules are located between the smectic layers.

We have demonstrated that the X-ray anomalous dispersion technique is quite useful to determine the positions of dopant molecules in soft matters.

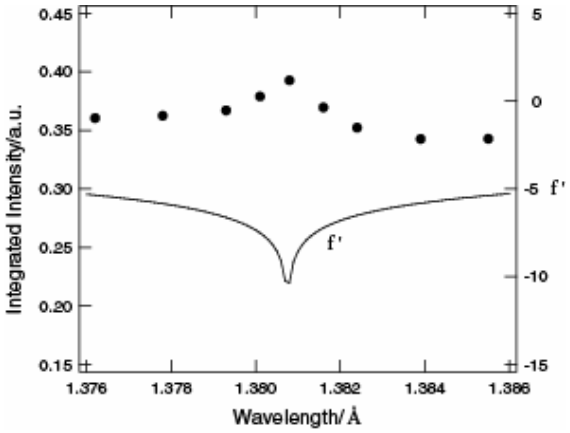

Fig. 1. Wavelength dependence of the integrated intensity for the 001 reflection (circles) and the real part f' (a solid line).

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