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Structure Analysis of Smectic Liquid Crystal with Metal Complex Using X-ray Anomalous Dispersion Effect

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Introduction

The knowledge of the location of guest elements, which are added into host substance, is of importance in studying their interaction between them in soft matters. Among the various methods, small-angle X-ray scattering (SAXS) with the X-ray anomalous dispersion effect is a very powerful technique for revealing such a structural formations in the size range of nanometers. The theory of this method is based on the energy dependence of the scattering factors of the different atoms which are complex quantities. We can distinguish the guest and host molecules by measuring the scattering intensity around the absorption edge of the guest elements. We have made an attempt to determine the location of Cu and Zn elements doped into a smectic liquid crystal with layered structure in this report.

Experimental

We used poly(oxyethylene) cholesterol (POE) exhibiting the smectic A phase, copper and zinc salt (CuM and ZnM). Measurements were made in a 1% CuM-doped POE and ZnM-doped POE. The SAXS measurements were carried out at BL10C of Photon Factory of KEK. SAXS intensities were measured as a function of the X-ray energy around the Cu absorption edge between 8.96-9.00 keV and the Zn absorption edge between 9.64-9.68 keV with an energy step of 5 eV, respectively. 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 with the reflections with 00*l*. Fig. 1 shows the energy dependence of the integrated intensity of the 001 reflection in CuM-doped POE and ZnM-doped POE. For a simple model that guest 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_k and n_k are, respectively, the Fourier transforms of the electron density of the smectic liquid crystal and the averaged number density of the guest atoms, and f is the atomic form factor of guest atom. Note that in the smectic liquid crystal we can take ρ_k and n_k as real numbers. Around the absorption edge, the real part, f' , decreases, whereas the intensity increases at this point as shown in Fig. 1 (a) and (b). From these results and the second term of eq. (1), $\rho_k\ n_k$ (***k*** 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 guest molecules are located between the smectic layers.

We suggested that a small amount of Cu and Zn elements can be used as a probe through the X-ray anomalous dispersion technique.

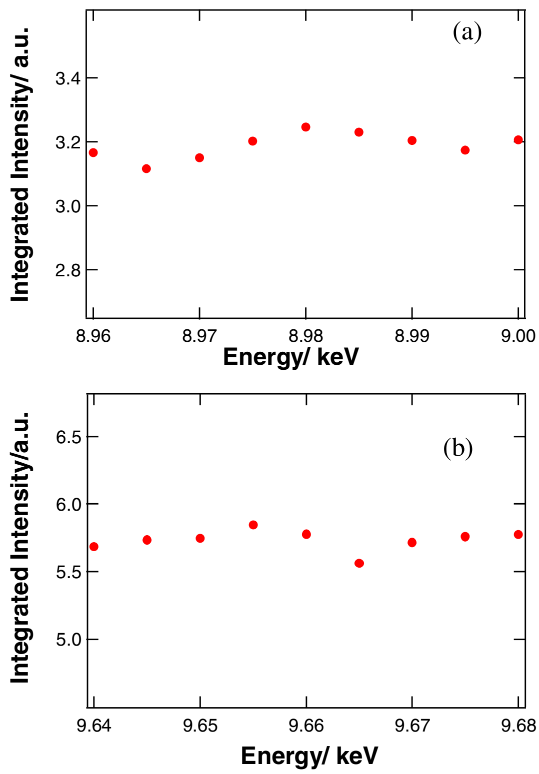

Fig. 1. Energy dependence of the integrated intensity for the 001 reflection of (a) CuM-doped POE and (b) ZnM-doped POE.

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