Investigating electron density of gyroid structures by X-ray diffraction

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To investigate the structure of nanoscale gyroid-like materials, it is essential to visualize the electron density. My collaborators and I have been developing a method to determine the electron density of gyroid phases of lyotropic liquid crystals by X-ray diffraction using monodomains (single-crystal regions). This method has enabled us to determine the electron density with unprecedented accuracy. Here, I will show the interface structure of the lyotropic liquid crystal gyroid phase revealed by the method. I also report the solution of the phase problem in the X-ray diffraction method.

In the gyroid phase of lyotropic liquid crystals, a microphase separation occurs between polar and nonpolar regions. The parallel surface (PS) model parallel to the gyroid surface and the constant mean curvature surface (CMCS) model were known as the interface structure. We investigated these interfacial structures for the gyroid phases of type I and type II lyotropic liquid crystals composed of amphiphilic molecules and water by single-crystal X-ray diffraction (ref. 1). For the observed X-ray diffraction data, we optimized the diffraction intensities expected from the two interface models. The PS model was clearly in better agreement with the observed data than the CMCS model. Judging from the degree of agreement, the interface is not in an intermediate state between the two models, but rather, it is much closer to the PS model. Figure 1 shows the electron density reconstructed from the amplitudes of the structure factors calculated from the observed intensity data and the phases calculated from the model. The high electron density (yellow) region of is the polar region, and a slightly lower density (orange) region locates near the center of the polar region. The electron density is slightly lower in the water-rich region within the polar region.

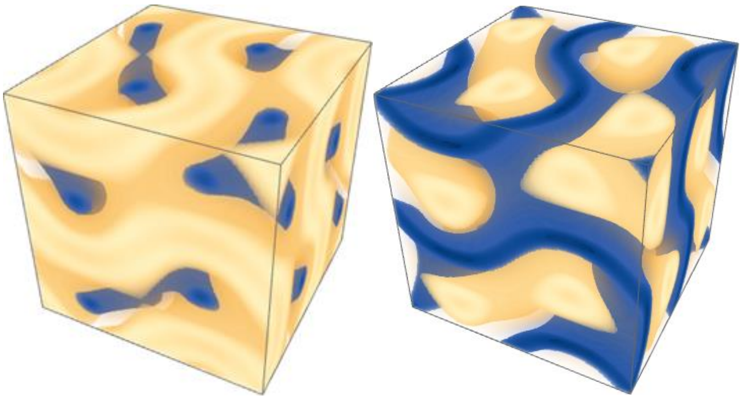

Figure 1 Electron density of lyotropic liquid crystal gyroid phases. (Left) Type I, (Right) Type II. Yellow and blue are high and low electron density regions, respectively.

To determine the electron density from diffraction data, it is necessary to retrieve the lost phase information of the structure factor. This is called the phase problem. I have developed a phase retrieval method applicable to bicontinuous liquid crystal phases including gyroid phase (ref. 2). First, I found two indicators of the characteristics of bicontinuous liquid crystal phases that appear in the electron density. I found that electron densities with small indicator vaclues tend to be the correct solution. I then developed an algorithm to find the correct electron density. Using these methods, the electron density of bicontinuous liquid crystal phases such as a gyroid phase can be easily obtained from diffraction data only. Using this method, we were also able to construct a new structural model of the chiral cubic phase of thermotropic liquid crystals (ref. 3).

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