Measuring the Orientational Distribution Function of Nematic *fd* Virus Using Small-Angle X-ray Diffraction

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Introduction

The simplest model of a liquid crystal treats the molecules as hard, rigid rods. In colloidal systems, interparticle potentials are dominated by steric repulsions. For a dilute system of long rods, Onsager developed a theory for the free energy[1] that shows a competition between the entropy of packing, which is maximized when the particles are aligned, and an entropy of mixing, which is maximized when the particles are randomly oriented. This competition produces a first-order phase transition from an isotropic to a nematic phase. Using x-ray diffraction, it is possible to measure the orientational distribution of the rod-like colloids in the nematic phase.[2]

Methods and Materials

Rod-like viruses have maintained their position as the most promising experimental system, because nature has created them to be monodisperse. Genetic engineering of viruses to create a homologous series of rods varying only in length is a standard procedure in molecular biology, and thus makes viruses an ideal system to study rod-like phase behavior. The *fd* virus was suspended in different ionic strength buffers. Samples were sealed in quartz capillaries, and aligned with a 2-T permanent magnet to form a monodomain nematic liquid crystal. The x-ray beam was monochromatic with an energy of 7.664 KeV.

Preliminary analysis was done using the methods of Meyer et al.[2] The equation that relates the scattered intensity to the orientational distribution function (ODF) of the nematic phase is $I(\psi)=\int f(\Gamma) I_s(\omega) d\omega$, where $I(\Psi)$ is the intensity distribution at a constant radius, $f(\Gamma)$ is the ODF, and $I_s(\omega)$ is the single particle scattering intensity. $\omega=\sin^{-1}(\cos(\Gamma)/\cos(\psi))$, and is the angle between rod and incident beam. The order parameter, S, is calculated from $S=\int f(\Gamma) P_2(\cos(\Gamma)) d\Gamma$, where P_2 is the second Legendre polynomial. Because the ODF is unknown it was approximated as a Gaussian and fit to the data.

Results and Discussion

In our preliminary analysis the interparticle interference peak and the equatorial form factor peaks were analyzed. At low concentrations, when layer lines began to overlap due to a high degree of orientational disorder, analysis of the form factor peak was no longer possible using this method.

From our data, we have been able to determine that there is a systematic concentration dependence of the order parameter at both the interparticle and intraparticle scattering peaks (Figs. 1 and 2). This trend appears to be independent of ionic strength.

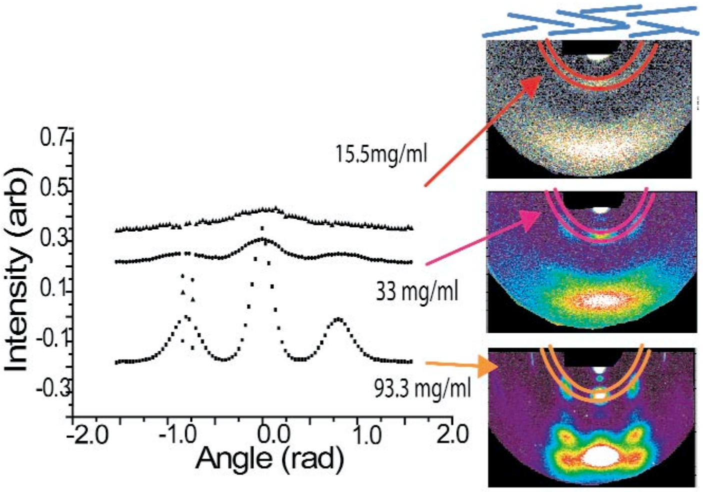

FIG. 1. Scattered intensity as a function of angle from the innermost intraparticle peaks. As the concentration of fd *rods increases, the alignment of the nematic increases and the peaks become more defined. The cartoon above the diffraction images indicates the orientation of the rods. The interparticle interference peak is just outside the beam stop. Angular scans of the 2D diffraction data are on the left. The scattered intensity in these scans arises from the form factor.*

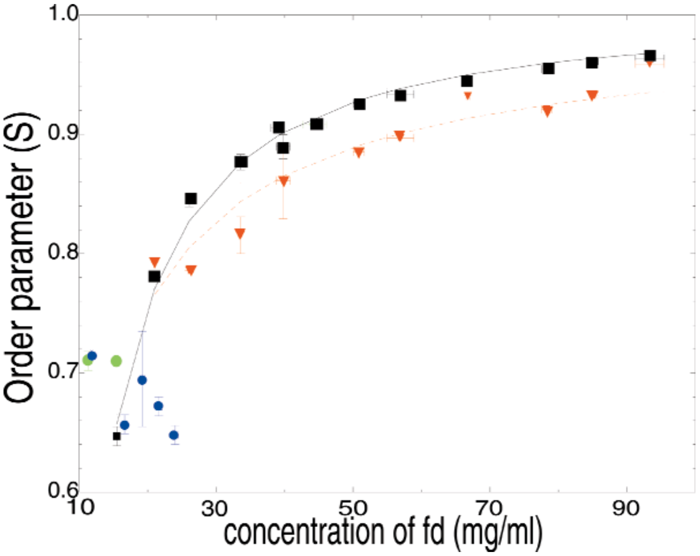

FIG. 2. Concentration dependence of the order parameter. The lower curve is from the equatorial intraparticle peak. The upper curve is from the interparticle interference peak. Circles are at the I-N coexistence concentration. The I-N samples vary in ionic strength.

The calculated S from both the intraparticle scattering and the interparticle interference peak agree in form and even in value for high concentration. It is surprising that the two values for S were not consistent at low concentrations. It is unclear if this difference in S is a result of error due to background from the detector and lack of angular range in the intraparticle scattering peak, or where it is a result of the interparticle interactions intrinsic to the peak in the structure factor.

Though the interparticle peak yielded angular intensity distributions with very precise Gaussian fits, we are hesitant about the accuracy of those results for the ODFs and corresponding order parameters because the scattered intensity contains correlations from interparticle interactions. Analysis is underway to calculate the ODF from the intraparticle scattering, accounting for the overlapping layer lines at low concentration.

Acknowledgments

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