Colloidal Crystallization of C_{60}/Polymer-Grafted Silica Particles in Organic Solvent

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Determination of inter-sphere distance

Inter-sphere distance (d_{cal}) in colloidal crystals was calculated from volume fraction (ϕ) on assumption of face centered cubic (fcc) closed packing by Eq. (1) [33], induced as follows.
The relation of number of sphere particles per mean size of single crystals, N_c, with volume of single crystals (L^3) is given for the cubic lattice by

$$L^3 = \frac{1}{\sqrt{2}} N_c {d_{cal}}^3 . \quad \text{(S1)}$$

Volume fraction of particles (ϕ) is presented by

$$\phi = \frac{N_c (4/3)\pi (r/2)^3}{L^3} \quad \text{(S2)}$$

where d is diameter of the particle.
From Eqs. (S1) and (S2), Eq. (1) is obtained,

$$d_{cal} = 0.9047 \times r \div \phi^3 \quad \text{(1)}$$

The inter-particle distance (d_{obs}) was also determined by the wavelength at the peak-top by combining Bragg's law and the relationship between lattice constant d and inter-particle distance d_{obs}. The relationship, $d = \sqrt{\frac{2}{3}} d_{obs}$, holds for close-packed lattice, either face-centered cubic (fcc) or hexagonal (hcp), with hexagonally ordered planes parallel to the interface. The relation between inter-particle distance, d_{obs}, and the wavelength at peak-top, λ_p, was presented by the following modified Bragg equation [1] by assuming fcc or hcp structure of colloidal crystals:

$$\lambda_p = 2d\sqrt{n^2 - \sin^2\theta} \quad \text{(S3)}$$

where n is the refractive index of solution. In this case, the reflection spectra were measured at the 90^o position from the cell surface by a spectral analyzer. Therefore, d_{obs} is obtained by following Eq. (2),

$$d_{obs} = \sqrt{\frac{3}{8}} \frac{\lambda_p}{n} \quad \text{(2)}$$

Where the refractive index, n, of the solution was presented as the average of solute (polymer-grafted colloidal silica) and solvent as follows:

$$n = \phi \times n_{silica} + (1-\phi) n_{sol}$$

where n_{sol} is the refractive index of solvent (1.34411 for acetonitrile at 293 K) and n_{silica} is the refractive index of silica, 1.50. The change of refractive index by polymerization was not considered

in the calculation because the refractive index change cannot be obtained for each step.

Reference

1. Hiltner, P A, Krieger, I M (1969) Diffraction of Light by Ordered suspensions. J Phys Chem 73, 2386-2389.