061108 Quiz 7 XRD

1) Scattering from any object in small angle can be described in terms of an average size, the radius of gyration, Rg, through the Guinier function,

$$I(q) = Nn_e^2 \exp(-q^2 R_g^2/3). = K \exp(X^2/2\sigma^2)$$

where $X = q$ and $s^2 = 3/(2R_g^2)$. What kind of function is Guinier's law?

2) The Fourier transform of an exponential is an exponential in the paired Fourier parameter, i.e. "r" in this case. Explain in real space why the kind of function you mentioned in part 1 can explain the pairwise correlation function for any object in the small-angle regime. (You may want to compare a protein in a crystal to a protein in solution in this answer.)

3) Atoms of a given type are indistinguishable while objects on the colloidal/nanoscales have a distribution in size and shape. How can this effect the difference between scattering in the XRD range of angle and scattering at small-angles. (Give an example of an object on the colloidal or nanoscale).

4) The diffusion of atoms is extremely rapid with the mean free path (average translation) of about 0.1 mm or one million times their size, while colloids move slowly with mean free paths on the order of their size at best. Explain how this effects the difference between XRD and small-angle scattering.

5) In lab we measured small-angle scattering from lamellar crystals in polymers. Explain how the polymer chain and the polymer unit cell build up this stacked lamellar structure. (Draw sketches to show how the unit cell and chains fit into the lamellar crystals and explain why the lamellae tend to stack.)

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1) This is a Gaussian function with a mean of q = 0 that describes a bell-shaped curve or normal distribution about q = 0 for a random distribution.

2) The protein in a crystal is fixed in orientation relative to other proteins in the crystal. When a solution is made of this crystal, the protein is free to rotate and translate rapidly so that a SAXS pattern will observe a smeared structure. Further, the calculation of the pairwise correlation function involves taking a random starting point in a particle (which is already randomized by rotation and translation) and measuring the probability that a point in an arbitrary direction from this starting point is also in the particle. This serves to further smear out the structure. Any structure, regardless of shape will display a radius of gyration. The radius of gyration is the moment of inertia using electron density as a weighting factor.

3) It is not possible to organize colloidal structures into a real crystal with long range order. It is also difficult to impossible to arrange nano-scale structures in a real crystal. This is due to imperfections in structure and due to the lack of a real thermodynamic equilibrium for large objects. For example, sand on the beach has similar grain sizes but will never form a crystal structure with long range order. This means that only a few structure factor peaks will be possible (usually only one) in small angle scattering and that the diffractions peaks will be extremely broad due to disorder and irregularity of the structural units.

4)   Colloids can't really form crystals from a kinetic perspective even if they had perfect structure. They can't probe enough arrangements due to slow motion to find an energy minimum on any reasonable time scale. This means that the structure factor will be dominated by defects and disorder despite some tendency to form crystals.

5)
http://www.eng.uc.edu/~gbeaucag/Classes/MorphologyofComplexMaterials/Chapter2html/Chapter2.html
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