Answer THREE questions

The numbers in square brackets in the right-hand margin indicate the provisional allocation of maximum marks per sub-section of a question.

1. (a) By considering a plane x-ray wave incident on an element of charge at a vector position $\mathbf{r}$ from an origin, show that the phase difference of the scattered beam with respect to the scattering from the origin is given by

$$(\mathbf{k}' - \mathbf{k_0}).\mathbf{r},$$

where $\mathbf{k_0}$ and $\mathbf{k}'$ are vectors representing the direction and wavelength of the incident and scattered x-ray respectively, with $|\mathbf{k}'| = |\mathbf{k_0}| = 2\pi/\lambda$, and λ is the x-ray wavelength. [6]

(b) Sketch the scattering diagram representing the above scattering situation, showing the scattering angle 2θ and scattering vector $\mathbf{K} = \mathbf{k}' - \mathbf{k_0}$. What is the magnitude of $\mathbf{K}$? [4]

(c) A white beam of x-rays, with wavelengths between 0.5Å and 1.5Å, is incident on a single crystal of a primitive cubic material. The smallest scattering angle observed is $2\theta = 5.73°$. Using the Bragg equation, calculate the unit cell parameter. [5]

(d) A polycrystalline powder of the same material is now used in a white beam powder diffraction experiment. Estimate the number of reflections you might see in this experiment. [5]

2. (a) Write down an expression for the structure factor of a crystal, explaining the meaning of the terms that appear in your expression. [3]

   (b) Show that, for a body centred cubic lattice, only those reflections are observed for which $h + k + l$ is even. Explain the physical reason for the absence of the other reflections. [7]

   (c) A powder diffraction experiment on a cubic crystal, using monochromatic x-rays with a wavelength of 1.0Å, shows the first eight powder lines at the following scattering angles:

   $19.2°, 27.3°, 33.6°, 38.9°, 43.8°, 48.2°, 56.3°, 60.0°.$

   Deduce the Bravais lattice type. [4]

   (d) If you were to use a monochromatic neutron beam of the same wavelength for this experiment instead of x-rays, how might you expect your diffraction pattern to differ from that observed using x-rays. [3]

   (e) KCl is known to have a face-centred cubic lattice structure. However, inspection of the sequence of powder diffraction lines from an x-ray experiment suggests it is simple cubic. Explain this apparent discrepancy, and why you would be unlikely to have been led astray if you had used neutrons. Note that the atomic numbers of the chlorine and potassium atoms are 17 and 19 respectively. [3]

3. (a) Sketch the kind of diffraction patterns (expressed as scattered intensity against scattering angle or scattering vector) you would expect to see for (i) a poly-crystal, (ii) a glass, and (iii) a liquid of the same material, all measured in Debye-Scherrer ('powder') geometry. [3]

   (b) Explain how these three 'phases' differ in terms of both their molecular structure *and* motions. [6]

   (c) Explain how we can describe quantitatively the structure of a liquid or a glass in terms of a function such as a radial distribution function. How can we extend this description for a binary liquid containing two different atoms? [5]

   (d) In a diffraction experiment on a liquid, we measure the intensity scattered as a function of scattering vector $I(\mathbf{K})$, and essentially Fourier transform this to obtain a radial distribution function. However, if we have a binary liquid such as molten nickel chloride, our resulting radial distribution function does not distinguish between the nickel and the chloride centres in the liquid. Describe how you might modify your diffraction experiment to find out how the chloride ions are arranged in the neighbourhood of the nickel ions. [6]

PLEASE TURN OVER

4. (a) List and explain two advantages of neutrons over x-rays for studies of structure and dynamics of condensed matter. [4]

(b) Describe x-ray or neutron scattering experiments that could solve *four* of the following problems. In each case, as well as specifying why you are using x-rays or neutrons, describe the *nature* of your sample, show the general arrangement of the scattering experiment, and describe the kind of information you expect to obtain.

    i. The structure of crystalline sodium chloride.

    ii. The structure of the high temperature superconductor $YBa_2Cu_3O_{7-x}$, with particular reference to the oxygen structure.

    iii. The structure of the molecule of C_{60} ('buckyballs').

    iv. The structure of a surfactant at an air-water interface.

    v. The location of the nucleic acid in the foot and mouth disease virus. [16]

5. (a) Describe what you understand by a *colloid*. Give three examples from your own experience, stating the components in each. [8]

(b) Calculation of the van der Waals forces between colloidal particles shows normally an attraction between the particles. Yet experience shows that colloidal systems are often stable against particle aggregation. Explain how a colloidal system can be stabilised in solution by adding a flexible polymer to the solution, paying particular attention to the thermodynamic reasons for the stabilisation. How, and why, would the effectiveness of the colloidal stabilisation be affected if the stiffness of the polymer were increased? [7]

(c) For a colloidal system of spheres of radius R, the (attractive) potential energy between two spheres separated by a distance H is given by

$$u = -AR/12H,$$

where A is the Hamaker constant. If we heat up this system, there should come a point at which the thermally induced fluctuations should be sufficient to overcome the tendency of the spheres to aggregate under the attractive forces. For $R \sim 100$nm, and a typical Hamaker constant for an aqueous system of about 10^{-20}J, estimate the temperature necessary to give rise to sufficient thermal energy to counteract the attraction. Take Boltzmann's constant to be 1.38×10^{-23}JK^{-1}.

In the light of the temperature you obtain, comment on the possible viability or otherwise of temperature stabilisation of aqueous colloids. [5]

END OF PAPER