Part III Experimental and Theoretical Physics

Frontiers of Experimental Condensed Matter Physics

Work Sheet for Supervision 1

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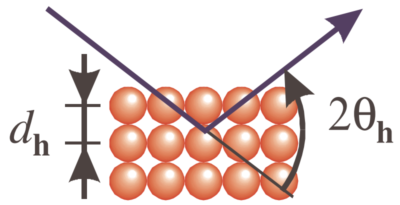
1 In a time-of-flight neutron powder diffractometer, a sharp pulse of neutrons with a range of wavelengths is fired at the sample. The diffracted signal is measured at a fixed scattering angle 2θ, where Bragg's law relates the scattering angle, for a particular reflection, **h**, to the separation of the corresponding planes, $d_{\mathbf{h}}$, through $\sin\theta_{\mathbf{h}} = \lambda/2d_{\mathbf{h}}$ (see diagram for definition of $\theta_{\mathbf{h}}$)



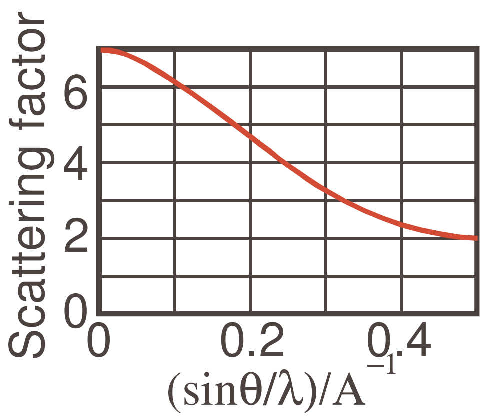
The diffraction pattern comes from measurements of the time taken for the neutrons in a single pulse to travel a flight path of distance, l, from the source to the detector. Show that d and l are related by

$$d = ht/2ml\sin\theta,$$

where m is the mass of the neutron and h is Planck's constant.

An experiment aims to determine d as accurately as possible. Take the uncertainty in d due to a parameter x, say, as $\Delta d = \Delta x(\partial d/\partial x)$. Show that the optimum choice of θ corresponds to a backscattering geometry. The uncertainty in l arises from the length of the neutron moderator, which can be taken as 2 cm. Determine the flight path necessary to give $\Delta d/d = 10^{-3}$ and $\Delta d/d = 2x10^{-4}$, which correspond to the moderate resolution instrument POLARIS, and the high resolution instrument HRPD at the ISIS spallation source (see: www.isis.rl.ac.uk). (Ans: 20m, 100m)

2. The atomic scattering factor for a nitrogen atom is shown in the figure below:



Consider two nitrogen atoms at positions r = (0.5, 0, 0)Å, with an incident beam of x rays, λ = 1.54Å, along the vector direction [1, 0, 0]. Sketch the scattered intensity in

the x-y plane. For the scattering vector $\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$, show that $|\mathbf{Q}| = 4\pi \sin\theta/\lambda$, where θ is defined as in Q.1. For scattering at angles of (a) 2θ=40° and (b) 2θ=80° in the x-y plane, calculate the modulus of the scattering vector, and hence the vector **Q**. Determine the scattering amplitude, within the kinematic scattering approximation, for the two angles.
(Ans: (a) Q=(-0.954,2.623); $F = f(\sin\theta/\lambda)\times[\exp(i\mathbf{Q}.\mathbf{r}_1)+\exp(i\mathbf{Q}.\mathbf{r}_2)]$ = 4.4x1.77 = 7.79; (b) Q=(-3.37,4.02); $F = f(\sin\theta/\lambda)\times[\exp(i\mathbf{Q}.\mathbf{r}_1)+\exp(i\mathbf{Q}.\mathbf{r}_2)]$ = 2.2x(-0.228) = -0.502)

3. In Q. 2 scattering occurs in all directions. How is the situation changed if, instead of a single, rigid molecule, there is:
(a) a square, 2-D lattice of molecules in the x-y plane (lattice constant 2.0Å)
(b) a single molecule, which vibrates (Sketch the correlation function and discuss the scattering)
(b)a single atom, which hops randomly from site to site on the same square lattice. (Sketch the correlation function P(x,t), for one spatial dimension and make an argument that scattering into the Bragg peaks of the lattice is necessarily elastic while the scattering in other directions is inelastic)

4. Write short essays (~2 sides of handwritten A4) on:
(a) A comparison of elastic scattering by electrons, neutron and x-rays, explaining how experiments using these probes provide complementary structural information.
(b) Thermal effects in diffractive scattering.

5. Measurements for copper metal give the mean-squared displacements of the atoms from their average positions as 0.021 Å^2 at 293 K, and 0.096 Å^2 at 1273 K. Copper has a cubic close-packed (f.c.c.) structure with a = 3.615 Å. Estimate the ratios of the intensities at the two temperatures of (a) the lowest-angle and (b) highest-angle reflections that can be measured with Cu Kα radiation, λ = 1.54Å.

6. For the surface phonon measurements illustrated in the lectures, consult the original paper (Phys Rev **B58** (1998) 13264) and determine the phonon wavevector of the Rayleigh peaks in Fig. 4a. Hence estimate the speed of sound in this material.