

Soft condensed matter physics I, spring 2010

Exercise 1

The answers are to be returned no later than Tue 2.2.2010 at 16:00. The answers are discussed in the exercise session Thu 4.2.2010 at 16:00, room D115.

Crystallography, structural organization and x-ray diffraction.

1. a) There are 7 possible crystal systems. Name them all and state the minimum symmetry elements that define them. (1 p.)
b) Suppose a simple rectangular (2D) lattice. Sketch the planes corresponding to Miller indices (010), (110), (230) and $(\bar{1}10)$. (1 p.)
c) What are the 3 Bravais lattices in the cubic system? Sketch planes (100), (110) and (111). (1 p.)

2. a) What is the coordination number for 1) infinite 1D linear chain 2) infinite simple rectangular 2D lattice and 3) infinite 3D bcc lattice.
b) Calculate the number of particles needed in a 1D linear chain to get a coordination number of 1.6. How about 1.9? (1 p.)
c) Sketch the RDF (radial distribution function) of an ideal hcp crystal up to the 4th coordination shell as a function of lattice constant a . (1 p.)

3. The classical formula in the theory of x-ray scattering gives the amplitude of radiation scattered by the point M (Fig. 1)

$$A \propto f \exp \left[-i \frac{2\pi}{\lambda} (\mathbf{s} - \mathbf{s}_0) \cdot \mathbf{OM} \right],$$

where f is the scattering factor of point M , 2θ is the scattering angle, λ is the wavelength of radiation and \mathbf{s} and \mathbf{s}_0 are unit vectors. Using the geometry shown in Fig 1,

- a) Show that the length of the scattering vector \mathbf{q} is (2 pts.)

$$q = \frac{4\pi \sin(\theta)}{\lambda}.$$

- b) Why is it convenient to express the scattering in units of q [$1/\text{\AA}$] instead of scattering angle 2θ [$^\circ$] (1 pt.)?

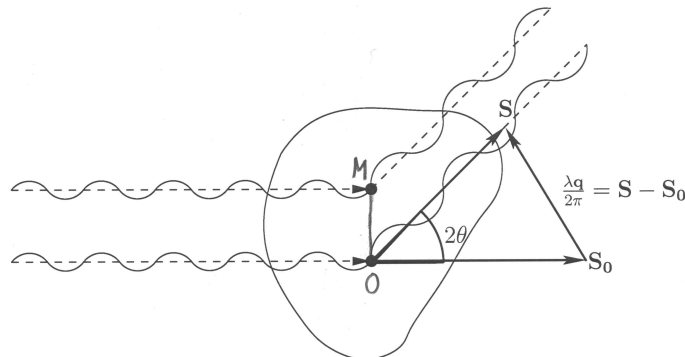


Figure 1: Scattering from a single particle.

4. The Scattering intensity is related to the *form factor* $f(q)$ of the scattering particle (i.e. $I(q) = |f(q)|^2$). The form factor of an arbitrary electron density function $\rho(\mathbf{r})$ can be calculated as

$$f(q) = \int \rho(\mathbf{r}) \exp(i\mathbf{q} \cdot \mathbf{r}) d^3\mathbf{r}.$$

a) Calculate the form factor of a hollow homogenous sphere with an inner radius of r_1 and an outer radius of r_2 . (2 pts.)

b) Plot the scattering intensity of a hollow sphere between $q = 0 - 10$ [1/nm] with the following parameters:

1) $r_1 = 4$ nm; $r_2 = 10$ nm,

2) $r_1 = 6$ nm; $r_2 = 10$ nm and

3) $r_1 = 8$ nm; $r_2 = 10$ nm.

In the plots, please use linear q-axis and logarithmic intensity axis. Elaborate on the differences between the plots. (1 pt.)

5. *PowderCell computer program*. Download and install PowderCell from the link provided in the homepages of the course. The Powdercell structure file of cellulose-I β is also given in the homepages. Use PowderCell to answer the following questions.

Calculations are not required. Each answer is worth 1/2 points.

a) Use *File -> Load* to open the Cellulose-I β structure data. Using *Structure -> Edit initial data*: what are the lattice parameters of the unit cell of Cellulose-I β . Which crystal system cellulose-I β belongs to?

b) Plot the unit cell as 111-projection (*Structure -> Projection plane*). Print and attach the figure to your exercise paper. Which axis is the cellulose chain axis?

c) Calculate the powder diffraction pattern (*Diffraction -> Diffraction ON*). Make sure the wavelength of radiation corresponds to Cu K α_1 (*Diffraction -> Experiment*). What are the three strongest reflections?

d) Try (*Diffraction -> HKL - List*). What are the scattering angles (in 2θ [°]) of the three strongest reflections?

e) What lattice spacings d [Å] do they correspond to?

f) Change the radiation to Mo K α_1 . Compare the results to the values obtained from problem d) and e). What are the differences and why?

Recommended reading on the subjects at hand

Hook & Hall, *Solid state physics*, chapter 1.

Cullity & Stock, *Elements of x-ray diffraction*, chapters 2 & 4.

Als-Nielsen & McMorrow, *Elements of Modern X-ray Physics*, chapter 4.

Nishiyama *et al.*, *Crystal structure and hydrogen-bonding system in cellulose I β from synchrotron x-ray and neutron fiber diffraction*, J. Am. Chem. Soc. **125** (2002), 9074-9082.