WS16/17   Condensed Matter Physics I
Exercise 1.   Crystal Lattices & Diffraction

Date: 26/10/2016   Handover: 3/11/2016

Notice*: In solving the proposed exercises clearly motivate the passages to reach the result. **The use of clear and compact notation is greatly encouraged, as well as the systematic use of dimensional checks of the expressions and results**. When you are asked to "evaluate" something this means to provide a numerical evaluation of the expression. In this case, at times, it might be necessary to indicate a parameter whose explicit numerical value is not provided, i.e. $\omega_c = \mathbf{1}.76\,H$ (Gauss) Hertz. Otherwise specified, all the evaluations are to be given with 3 significant figures.*

1.1 Honeycomb lattice.   (10 pts)

Let us consider the 2D honeycomb lattice (see Figure 1). Let us indicate the atomic position at the base and the top of the vertical side of the hexagon as A and B.

1. The honeycomb lattice is a Bravais with basis. Which Bravais is that? Choose and indicate the Bravais primitive vectors ($\mathbf{a}_1$ and $\mathbf{a}_2$).
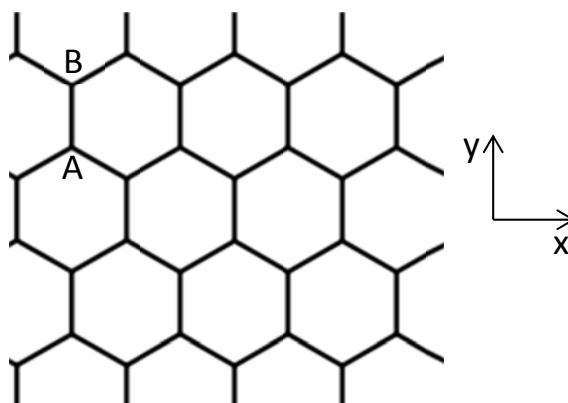

Figure 1: Honeycomb lattice.

2. Give the reciprocal of the Bravais lattice and its primitive vectors ($\mathbf{g}_1$ and $\mathbf{g}_2$).
3. Calculate the geometric form factor $F(\mathbf{G})$ relative to the generic reciprocal lattice vector $\mathbf{G} = n_1\mathbf{g}_1 + n_2\mathbf{g}_2$. Indicate with f_A and f_B the atomic form factors (consider them to be real numbers).

4. Give the general expression of the vector G for which $F(G)$ is real, independently from the value of the ratio f_A/f_B .

5. Consider now $f_A = -f_B$. Are there any G for which $F(G) = 0$? If so, indicate which and draw them on the reciprocal lattice.

1.2 Powder diffraction on C_{60} crystal.   (15 pts)

The solid C_{60} lattice is a face-centered cubic with conventional unit cell of side a.

1. Which is the corresponding reciprocal lattice? What is the side of its conventional unit cell?

2. In a powder diffraction experiment a C_{60} polycristal is placed at a distance L from a flat photographic film, and a monochromatic X-ray beam of wavelength λ is directed to the sample with an initial wavevector k_0 perpendicular to the film (See Figure 2). The projection Δx of the back-diffracted beams of wavevector k′ are recorded on the film and can be easily measured.

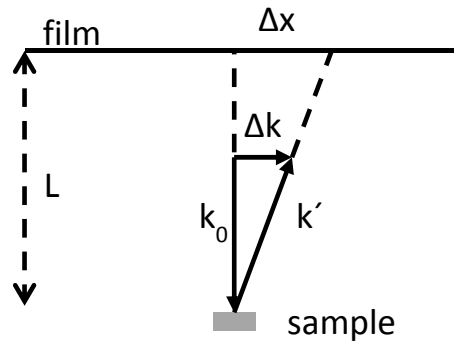Figure 2 : Powder diffrraction setup (schematics)

We know that the diffraction condition prescribes $\Delta k = k' - k_0 = K$ and that $|k_0| = 2\pi/\lambda$. Consider the approximation in which Δk is parallel to the film. Give the formula linking Δk, Δx, λ and L. Verify that $2\pi/\lambda\,\Delta k = L/\Delta x$.

3. The diffractogram of the sample of C_{60} is recorded in Figure 3. We see they form a square lattice. Assume that it records the diffraction spots relative to the $K = (h,k,0)$ plane of the fcc reciprocal lattice, with h and k even. Indicate l_{K_0} as the spacing of the observed square lattice, corresponding to the reciprocal lattice spacing of $K_0 = 4\pi/a$. Use the result found in the preceding point to obtain a relation linking $l_{\Delta k}$ and a. By directly measuring on Figure 3 the value of $8l_{K0}$ with a ruler evaluate lattice constant a with its uncertainity. Compare your result with the accepted value of a=14.11±0.02 Å. Consider L=6 cm, λ=1,542 Å and that the diameter of the film in Figure 3 is 12 cm.

4. Why it is suggested to measure 8 times l_{K0} and not just l_{K0}? Which feature of the difractogram ultimately limits the uncertainity of the lattice constant?

5. At a closer look at Figure 3 we see that the (2,0,0) diffraction peak is very weak. Assume that the charge distribution of a fullerene ball is represented by a surface charge on a sphere of radius R=3.5 Å: $\rho(\mathbf{r}) = A\delta(r - R)$. Here $r = |\mathbf{r}|$. After finding the value of the constant A in units of the electron charge e, calculate the form factor of the C_{60} molecule in this

approximation. Show that the form factor of the (2,0,0) peak is indeed much less than that of the (2,2,0) peak. (*Hint: to solve the integral consider transforming in spherical coordinates*)
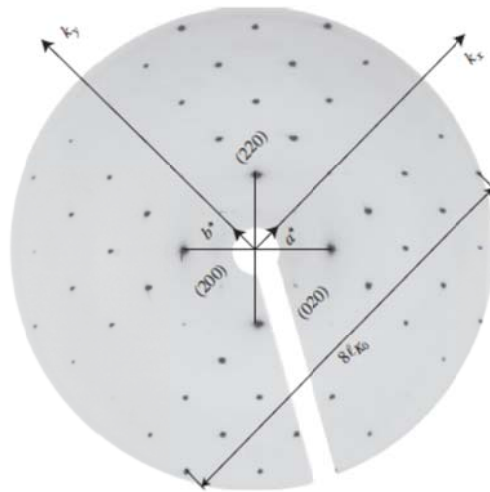

Figure 3: Powder diffractogram of C_{60}. The real diameter of the film is 12 cm.

1.3 Stripe order in a cuprate compound. (8 pts)

The common building block for most high temperature (high Tc) superconductors are copper oxide layers, as depicted in Figure 3(a). Considering a single isolated layer, assume the distance between copper atoms (filled circles) is a. In first approximation the layers have a fourfold symmetry; the crystal is tetragonal.

1. Sketch the Bravais lattice and indicate a possible set of primitive vectors for this crystal. What is the unit cell, and what is the basis?
2. In LaCuO4 once discovers, at closer inspection, that the CuO2 lattice is actually not flat, but that the oxygen atoms are moved a small amount out of plane ("up"and "down") in an alternating fashion [in Figure 3(b) ⊕ means up and ⊖ means down), forming diagonal striped undulations. What is the primitive cell and lattice spacing for the crystal? What is the reciprocal lattice? Describe (qualitatively) what happens in the X-ray diffraction pattern as the distortion is decreased gradually to zero. (*Hint: Sketch the corresponding Reciprocal lattices*)
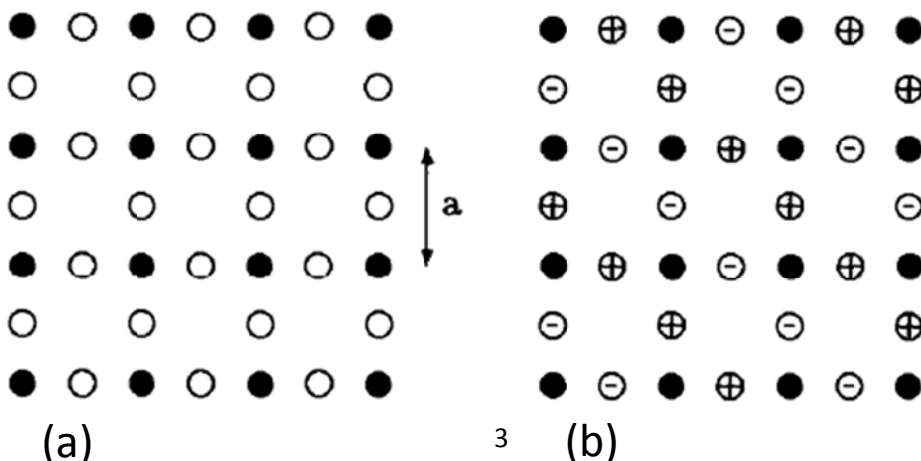

Figure 4 (a) CuO2 lattice; (b) distorted CuO2 lattice.