Solid State Physics
Exercise Sheet 3
Scattering and Diffraction

HS19
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Exercise 1 *Atomic form factor*

There is an atom in which the density distribution of one electron around the nucleus at the distance of $\vec{r}$ is given by $n(\vec{r})$.

1. Calculate the atomic form factor f as a function of the scattering vector $\Delta\vec{k}$
2. Derive a generalized equation for the structure factor S of an atom containing Z electrons

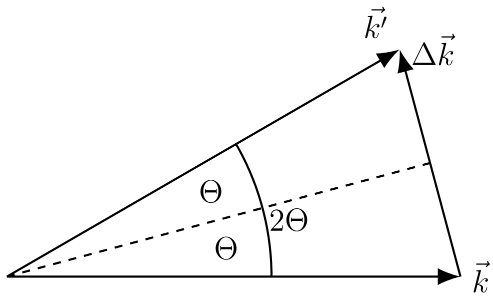

Figure 1: The scattering triangle.

Note that the scattering triangle (Figure 1) gives the relation between $\Delta\vec{k}$, the wavelength $\lambda = 2\pi/k$, and the scattering angle Θ:

$$\Delta k = 2\pi \frac{2\sin(\Theta)}{\lambda}. \tag{1}$$

Exercise 2 *Geometrical structure factor*

Calculate the structure factor S as a function of hkl for the GaAs structure with the assumption that the atomic form factors f are constant but different for Ga and As. What would happen if the two atoms had the same atomic form factor, as in the case of silicon/diamond?

Exercise 3 *Crystal structure of $BaTiO_3$*
Barium titanate crystallizes in a perovskite structure; i.e. a structure where the Ba atoms sit at the corners of a cube with a Ti atom at the cube's center and the O atoms in the centers of its faces (see Sheet #1, Exercise 3). Determine the intensity relationship between the (100), (110), (111) and (200) Bragg reflections assuming that $f_{Ba} = 7f_O$ and $f_{Ti} = 3f_O$.

Exercise 4 *Three phases of iron*
Iron can exist in three different phases that are all cubic, the α-phase (below 910°C), the γ-phase (between 910°C and 1403°C), and the δ-phase (between 1403°C and 1535°C). In powder x-ray diffraction experiments with a wavelength of 0.15418 nm, diffraction peaks were observed

- α-phase at 513K: $2\Theta = 44.67°$, 65.02° and 82.32°
- γ-phase at 1565K: $2\Theta = 42.66°$, 49.67°, 72.88° and 88.29°
- δ-phase at 1705K: $2\Theta = 43.72°$, 63.55° and 80.32°

1. Index all the diffraction peaks and determine the Bravais lattice of each phase
2. Evaluate the lattice constants of the three phases at the measured temperatures
   (Hint: remember the structures we observed for Sheet #0...)

Questions

1. In diffraction experiments, what does the (000) reflection correspond to?