University of Zurich[UZH]

Solid State Physics
Exercise Sheet 2

FS18
Prof. Dr. Johan Chang

TA: Stefan Holenstein

Due on 14^{th} March

Exercise 1 *Reciprocal lattice vectors*

In this exercise we prove some properties of reciprocal lattice vectors.

a) Show that a reciprocal lattice vector $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$ is orthogonal to the lattice plane (hkl).

b) Show that the distance d_{hkl} of two lattice planes with Miller indices (hkl) is given by

$$d_{hkl} = \frac{2\pi N}{|h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3|}. \tag{1}$$

What is the meaning of N?

Exercise 2 *Reciprocal lattice*

Calculate the primitive reciprocal lattice vectors $\vec{b}_1$, $\vec{b}_2$, $\vec{b}_3$ for

a) fcc and bcc lattices

b) the hexagonal lattice.

Exercise 3 *Ewald sphere*

Discuss qualitatively, using the Ewald sphere, what kind of interference pattern is observed in the diffraction of monochromatic light by linear point and line lattices.

Exercise 4 *Brillouin zone in the reciprocal lattice*

Construct the first four Brillouin zones for a two-dimensional simple rectangular lattice with $a_2 = 2a_1$.

Exercise 5 *Atomic form factor*

Calculate the atomic form factor f for a homogeneously charged sphere of charge Z and radius R as a function of Δk. Plot f as a function of $\sin(\Theta)$ if we assume $\lambda = R$. Calculate also $\lim_{\Theta\to 0} f(\Delta k)$.

Remember: The atomic form factor for an atom is given by its electron density distribution $n(\vec{r})$ (the charge density is $\rho(\vec{r}) = -en(\vec{r})$) according to

$$f(\Delta\vec{k}) = \iiint n(\vec{r}) e^{i\Delta\vec{k}\cdot\vec{r}} \mathrm{d}^3 r. \tag{2}$$

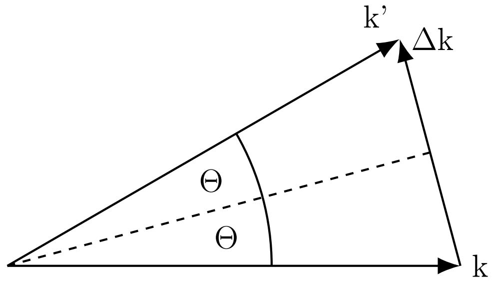

Figure 1: The scattering triangle.

Furthermore the scattering triangle (figure 1) gives the relation between Δk, the wavelength $\lambda = 2\pi/k$, and the scattering angle Θ:

$$\Delta k = 2 \cdot \frac{2\pi}{\lambda} \sin(\Theta). \tag{3}$$

Exercise 6 *Width of the diffraction maximum*

We assume that in a linear crystal on every lattice point $\vec{\rho} = m\vec{a}$, $m \in \mathbb{Z}$, there is an identical point-like scattering centre. The total amplitude of the scattered radiation is proportional to $F = \sum \exp\left(-im\vec{a} \cdot \Delta\vec{k}\right)$. The sum over M lattice points has the value

$$F = \frac{1 - \exp\left(-iM\vec{a} \cdot \Delta\vec{k}\right)}{1 - \exp\left(-i\vec{a} \cdot \Delta\vec{k}\right)} \tag{4}$$

when we use the series expansion

$$\sum_{m=0}^{M-1} x^m = \frac{1 - x^M}{1 - x}. \tag{5}$$

a) The scattered intensity is proportional to $|F|^2$. Show that

$$|F|^2 \equiv F^* F = \frac{\sin^2\left(\frac{1}{2}M\vec{a} \cdot \Delta\vec{k}\right)}{\sin^2\left(\frac{1}{2}\vec{a} \cdot \Delta\vec{k}\right)}. \tag{6}$$

b) For $\vec{a} \cdot \Delta\vec{k} = 2\pi h$, $h \in \mathbb{Z}$, a diffraction maximum appears. We change $\Delta\vec{k}$ slightly and define ε in $\vec{a} \cdot \Delta\vec{k} = 2\pi h + \varepsilon$ such that ε gives the first zero-crossing of the function $\sin\left(\frac{1}{2}M\vec{a} \cdot \Delta\vec{k}\right)$. Show that $\varepsilon = 2\pi/M$. What does this mean for the width of the diffraction maximum?

Exercise 7 *Structure factor*

Calculate the structure factor S as a function of hkl for the NaCl structure with the assumption that the atomic form factors f are constant but different for Na and Cl.

What would happen if the two atoms had the same atomic form factor? Which real material with NaCl-structure is close to this assumption?