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Fachbereich Physik

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Einführung in die Theoretische Festkörperphysik

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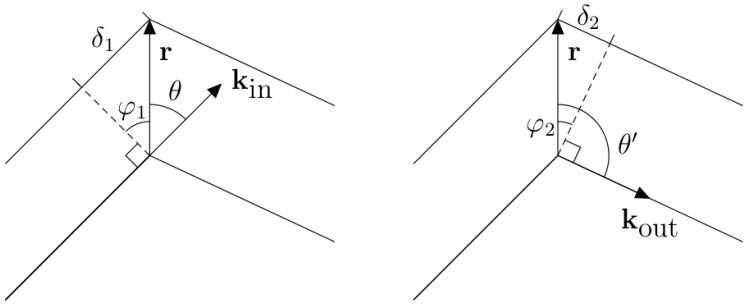
Exercise 2

(Due date: 04.11.2019)

Problem 1 (**Calculation of the structure factor**) (5 points)

We shine x-ray on a crystal and capture the scattered light with a detector. Since the x-rays are scattered at different points in the sample we see an interference pattern on the detector that stems from the different distances that each ray had to travel to the detector.

a) Calculate the phase difference between two waves where one wave was scattered in the origin and the other at the point $\vec{r}$. Use the values given in the figure below.



b) The scattering amplitude $F(\vec{K})$ after a single scattering (for simplicity we neglect multiple scattering processes) is obtained as an integral of the density multiplied with the phase difference over the volume of the sample. Show that the scattering amplitude can be written as

$$F(\vec{K}) = NS(\vec{K}), \tag{1}$$

where N is the number of unit cells in the sample,

$$S(\vec{K}) = \sum_{j=1}^{n_{\text{atom}}} f_j e^{-i\vec{K}\cdot\vec{r}_j} \tag{2}$$

is the so-called structure factor, n_{atom} is the number of atoms in the atomic basis and

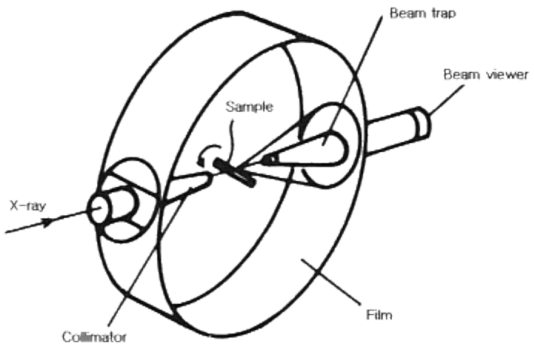
$$f_j = \int_V d^3r\, n_j(\vec{r}) e^{-i\vec{K}\cdot\vec{r}} \tag{3}$$

is the atomic form factor of the j-th atom at $\vec{r}_j$.

c) Calculate the structure factor of a simple cubic (sc), a body centered cubic (bcc), a face centered cubic (fcc) lattice and a zinc blende structure. You can assume that the crystals are composed of a single atom species and take all structures to be simple cubic lattices with a proper basis in the different cases. Where does the structure factor vanish?

Problem 2 (**Debye-Scherrer method**) (5 points)

The figure below shows the experimental setup that uses the Debye-Scherrer method. There, photons are scattered at a poly-crystalline sample and the resulting interference pattern is captured on a film.



In a Debye-Scherrer experiment with a cubic crystal we detect rings with the following angles:

$$2\theta_i = \{42.8°, 73.2°, 89.0°, 115.0°\},$$

where 2θ is the angle between the incoming and outgoing direction and i is the index of the interference ring.

a) Give an expression for the length of the reciprocal lattice vector, $\vec{K} = n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3$, of a simple cubic Bravais lattice, where n_j are integer, $\vec{b}_j$ are the basis vectors of the reciprocal lattice and a is the lattice constant.

b) Starting from the Laue condition derive an expression for $\sin(\theta_i)$ as a function of the so-called reflection index $N = n_1^2 + n_2^2 + n_3^2$. To each angle $2\theta_i$ belongs such an index N_i. Determine N_1, which belongs to the interference ring with the smallest diameter such that all N_i are integer.

c) Which cubic structure is compatible with experimentally determined data if the sample consist of a single atomic species? Use problem 3.1 and justify your answer.