UNIVERSITÄT SIEGEN
FESTKÖRPERPHYSIK

Crystallography (*winter term 2015/2016*)

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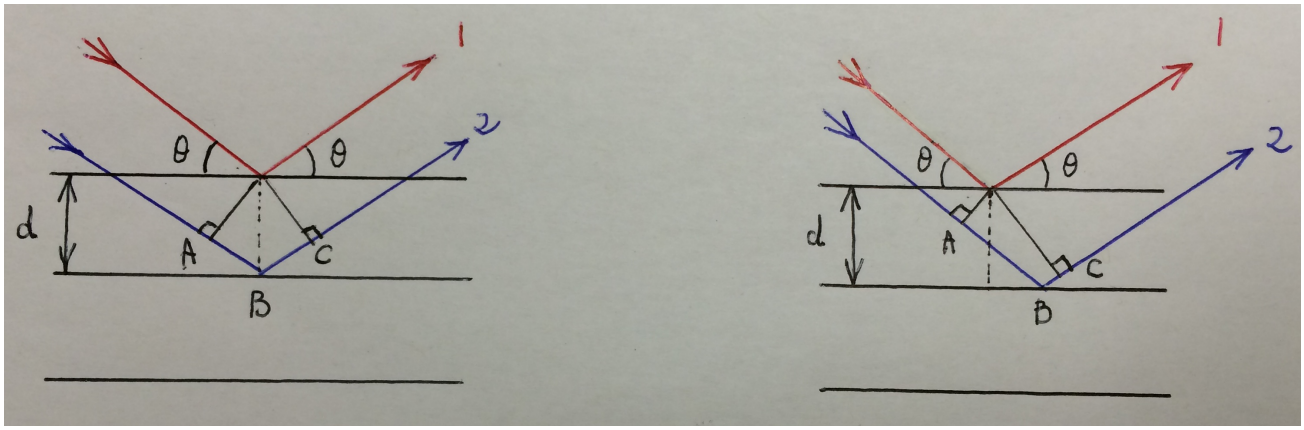
Exercise tutor: **Hyeokmin Choe** (ENC B-015)

Exercise sheet 9: Introduction to X-ray crystallography.

1. Bragg's law (5 points)

The figure below shows two different reflection geometries, which can be used for the derivation of Bragg's law. In both cases the path difference (AB + BC) between the wave 1 and the wave 2 must be calculated. Show that this path difference is the same for both geometries and equal to $2d \cdot sin\theta$.



2. Laue diffraction (8 points)

A single crystal of *quartz* (hexagonal crystal system, the lattice paraemetrs are a = 4.9Å, c = 5.4 Å) is investigated in a **white X-ray beam** (i.e. by means of the Laue method). The crystal is oriented so that the lattice basis vector, ***a***, points to the X-ray source. Your task is to reconstruct the above Laue experiment in the reciprocal space by:

a) Plotting 2D central section of the Ewald ball, so that the section is parallel to the lattice vectors ***a*** and ***b***. (the shortest wavelength of the X-ray spectra λ_{min} = 0.3 Å)

b) Plotting the lattice vectors ***a***, ***b*** and reciprocal lattice vectors ***a****, ***b****.

c) Plotting reciprocal lattice points *hk0* where *-4<= h,k < = 4* (you should get the reciprocal lattice consisting of 81 points)

d) Marking as **red those reciprocal lattice** points which give Bragg reflections on the Laue pattern, mark as **blue those reciprocal lattice points** which do not.

Choose any 3 of **red reciprocal lattice points** (free choice) and calculate the scattering angle (2θ) and the wavelength (λ) of the corresponding Bragg peaks.

3. Single crystal diffraction / Rocking curve (8 points)

A single crystal of $BaTiO_3$ (cubic crystal system, the lattice constant a = 4 Å) is investigated with a monochromatic Mo Kα radiation (wavelength λ = 0.71 Å). The crystal is initially oriented in such a way that the vector **a** is parallel to the incident X-ray beam. Your task is to construct the single crystal diffraction in reciprocal space by:

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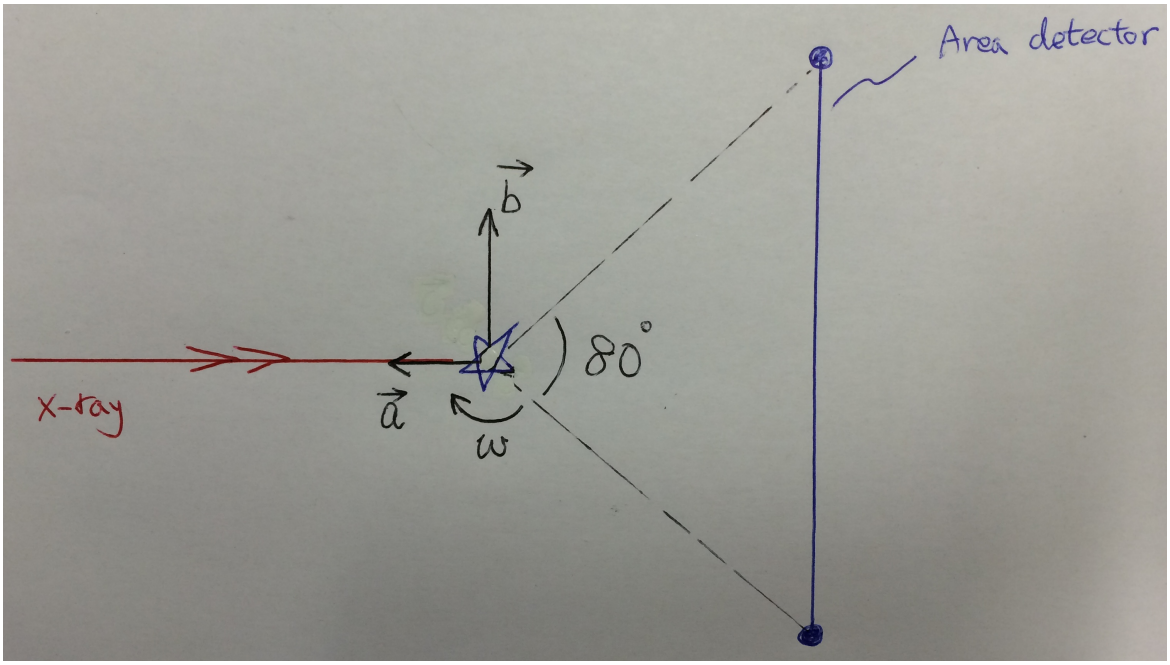
a) Plotting 2D section of Ewald sphere, so that the section is parallel to the lattice vectors **a** and **b**.

b) Plotting the lattice vectors **a**, **b** and reciprocal lattice vectors **a***, **b***.

c) Considering that the area detector covers 80°. How many Bragg reflections (l = 0) will be registered by the detector during the 35° of crystal rotation around the c-axis? Please find the indices $h\ k\ 0$ of the appearing Bragg reflections.



Please return on 01.02.2016