Excercises „Methoden Moderner Röntgenphysik II"

Date, Room and Time: 21. April 2009 , Seminarraum 5,   16:00-17:30

— Crystal Truncation Rods —

In Born-Approximation, the x-ray amplitude scattered by a crystal is given by

$$A(\vec{q}) \propto S(\vec{q}) \sum_{n_1=-M_1}^{N_1-1} \sum_{n_2=-M_2}^{N_2-1} \sum_{n_3=-M_3}^{N_3-1} \exp(i\vec{q}\cdot[n_1\vec{a}+n_2\vec{b}+n_3\vec{c}])$$

with the structure factor $S(\vec{q})$ the wave vector transfer $\vec{q}$ and the unit cell vectors $\vec{a},\vec{b},\vec{c}$. At infinity crystals all M_k and N_k are equal to infinity. At semi-finite crystals with a surface e.g. in the $\vec{a},\vec{b}$ -plane M_3 is a finite number e.g. $M_3 = 0$. For a cubic crystal and a variation of $\vec{q}$ along $\vec{c}$ (the z – axis) the $\vec{a}$ - and $\vec{b}$ -directions can be neglected. The problem becomes 1-dimensional.

1) Calculate the scattered intensity $I(q_z)$ of the Crystal Truncation Rod CTR for the 1-dimensional semi-infinity crystal with the interface at $M_3 = 0$ and finite but very large N_3.

Use $I(q_z) = |A(q_z)|^2$ and $\sum_{n=0}^{N-1} x^n = \frac{x^{N/2} - x^{-N/2}}{x^{1/2} - x^{-1/2}} \cdot x^{\frac{N-1}{2}}$

2) Make a sketch of $I(q_z)$ and explain the problems for $N_3 \to \infty$.

Introducing an absorption depth for the x-rays makes the calculations more realistic. The intensity of the x-rays in the depth z in an absorbing material follows $I(z) = I_0 \exp(-z/\Lambda)$ with the absorption length Λ.

3) Modify the scattered amplitude $A(q_z)$ of the Crystal Truncation Rod CTR for the 1-dimensional semi-infinity crystal with the interface at $M_3 = 0$ introducing the absorption effects to each of the components of the sum.

4) Using $N_3|\vec{c}| >> \Lambda$ and $|\vec{c}| << \Lambda$ (which is both usually the case) calculate the scattered intensity $I(q_z)$ of the Crystal Truncation Rod CTR for the 1-dimensional semi-infinity crystal with the interface at $M_3 = 0$ and finite but very large N_3 including absorption. Make a sketch and compare with the sketch of 2).

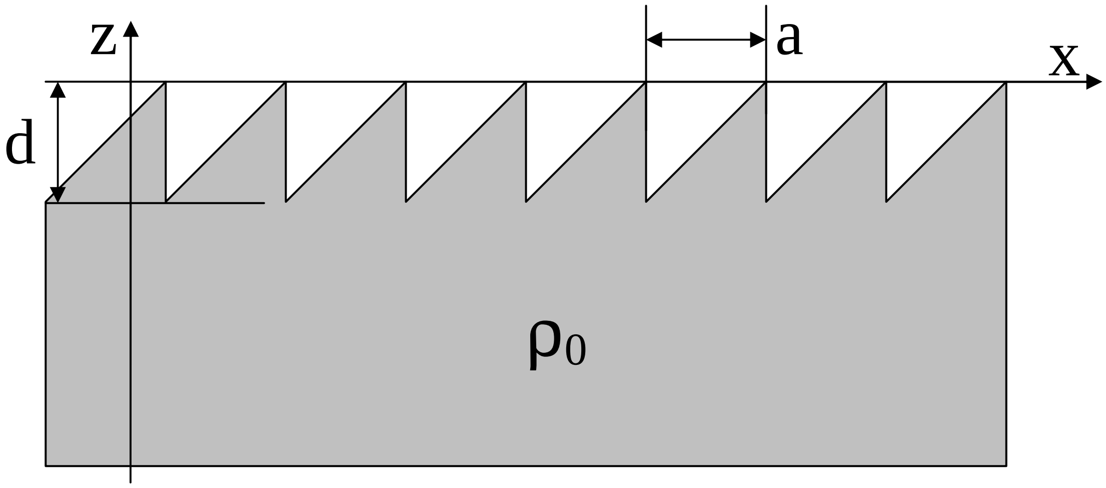
— X-Ray Reflectivity —

In Born-Approximation, the x-ray intensity reflected by a surface is given by

$$I(q_z) \propto \frac{1}{q_z^4} \left| \int_{-\infty}^{\infty} \frac{d\rho(z)}{dz} \exp(iq_z z) dz \right|^2$$

with the wave vector transfer q_z along z and the electron density profile $\rho(z)$ along z.

1) Calculate the reflected intensity of the following "sample surface with steps" by first generating the function $d\rho(z)/dz$ averaged over x.



2) Compare the result with a reflectivity of a one-layer system with substrate density ρ_0, film density $\rho_0/2$ and film thickness d.