

Excercises „Methoden Moderner Röntgenphysik II“

— 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 $N_3 \rightarrow \infty$.

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 $N_3 |\vec{c}| \gg \Lambda$ and $|\vec{c}| \ll \Lambda$ (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).