

Aufgabe 3-1:

Zinc-blend form of ZnS is cubic and has a lattice parameter of 5.41Å.

It has four zinc and four sulfur atoms per unit cell, located in the following position:

Zn: $\frac{1}{4} \frac{1}{4} \frac{1}{4}$ + face-centering translations,

S: 0 0 0 + face-centering translations

- Calculate the structure factor of the ZnS.
- Calculate the relative intensities of the first six lines on a Debye-Scherrer pattern made with Cu k_α radiation by considering the following equation.

$$I = |F|^2 P \left(\frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta} \right)$$

where F is structure factor, P is multiplicity and $\left(\frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta} \right)$ is Lorentz-polarization factor.

Aufgabe 3-2:

Debye-Scherrer pattern of tungsten (bcc) is made with Cu k_α radiation. The first four lines on this pattern were observed to have the following θ values:

Line	θ
1	20.3°
2	29.2
3	36.7
4	43.6

- Index these lines (i.e., determine the Miller indices of each reflection by the use of $\sin^2 \theta = \frac{\lambda^2}{4a^2} (h^2 + k^2 + l^2)$ and quadratic forms of miller indices)

$h^2 + k^2 + l^2$	2	4	6	8	10	12
hkl for body centered(bcc)	110	200	211	220	310	222

- Calculate their relative integrated intensities.