Aufgabe 4-1:

The temperature factor (e^{-2M}) in the intensity can be approximated to elements with cubic crystal structure:

$$M = \frac{1.15 \times 10^4 T}{A\Theta^2} \left[\phi(x) + \frac{x}{4}\right]\left(\frac{sin\theta}{\lambda}\right)^2$$

Where T the absolute temperature, Θ the Deby charachteristic temperature of the substance in °K, $x = \frac{\Theta}{T}$, and $\phi(x)$ is a function tabulated along with values of Θ (See Appendix 15)

Considering that the Cu and Pb have fcc lattice with lattice constant of 3.61Å and 4.95 Å, respectively.

(a) By what percentage the intensity of the highest-angle line on the diffraction pattern measured at 20° C with Cu kα radiation is reduced by thermal vibration of the atoms?

(b) Calculate the corresponding intensity reduction for 400 reflection lines of Cu and Pb measured at the same condition.

Aufgabe 4-2:

Debye-Scherrer pattern is measured from InSb powder using Cu kα radiation. The material

crystalizes in Zinc-blende structure with lattice parameter of 6.46Å.

(a) Determine the Miller indices of the first 3 lines in the pattern?

(b) Estimate the ratio of the integrated intensities of among these 3 Bragg reflections?

In and Sb atoms are located in the following position in a unit cell.

In: ¼ ¼ ¼ +fcc translation

Sb: 0 0 0 +fcc translation