

February 5, 2004

HOMEWORK NO. 4

Problem 1

For each of the following crystal structures, derive the structure factor and give the condition for constructive interference.

- (a) the rock salt structure,
- (b) the diamond structure,
- (c) the zinc blende structure.

Problem 2

A sample of chromium (BCC) was placed in an x-ray beam of wavelength 1.54 \AA . Diffraction from the (110) planes was obtained at $2\theta = 44.4^\circ$, where 2θ is the angle of diffraction. Calculate the lattice parameter of chromium.

Problem 3

Suppose you want to perform electron diffraction on an FCC crystal.

Sketch the following electron diffraction patterns which you would expect to obtain. Index the diffraction spots with the corresponding Miller indices.

- (a) 100
- (b) 110
- (c) 111
- (d) 211

Note: The $m_1 m_2 m_3$ electron diffraction pattern is obtained with the electron beam along the $[m_1 m_2 m_3]$ direction (i.e. the direction $\vec{R}_n = m_1 \vec{a}_1 + m_2 \vec{a}_2 + m_3 \vec{a}_3$) and shows the reciprocal lattice plane perpendicular to \vec{R}_n .

Problem 4

Shown in Fig. 1 is a plot of intensity against 2θ for an x-ray diffraction line. The Bragg angle is at $2\theta = 2\theta_B$. The intensity drops to zero at $2\theta = 2\theta_1$, as indicated in Fig. 1. Assume that the width of this diffraction peak is completely due to the finite size of the crystal. By using the Laue formalism, obtain an expression for $2\theta_1 - 2\theta_B$ in terms of the size of the crystal. Let the Miller indices corresponding to this diffraction line be m_1, m_2 and m_3 . Let the number of unit cells along the \vec{a}_1, \vec{a}_2 and \vec{a}_3 directions be N_1, N_2 and N_3 respectively. (\vec{a}_i are the fundamental translation vectors for the direct lattice). Give your answer for the case of a cubic lattice.

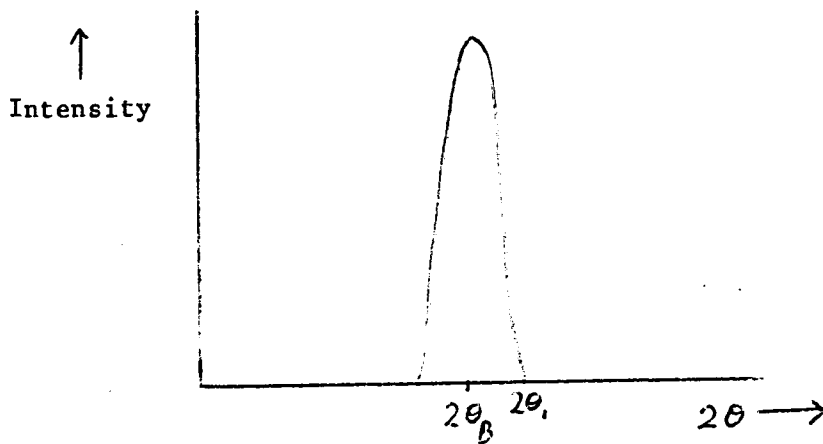


Fig. 1 The x-ray diffraction peak for a crystal

Problem 5

What is the minimum voltage that must be supplied to an x-ray tube to see diffraction spots from an aluminum crystal? Aluminum crystallizes in the FCC structure with lattice parameter $a = 4.05 \text{ \AA}$.

Problem 6

Determine, and list in order of increasing angle, the values of 2θ and (hkl) for the first three lines (those of lowest 2θ values) on the powder patterns of substances with the following structures, the incident radiation being Cu K α :

- (a) simple cubic ($a = 3.00 \text{ \AA}$),
- (b) simple tetragonal ($a = 2.00 \text{ \AA}$, $c = 3.00 \text{ \AA}$)
- (c) simple tetragonal ($a = 3.00 \text{ \AA}$, $c = 2.00 \text{ \AA}$)