STATE UNIVERSITY OF NEW YORK AT BUFFALO

Department of Mechanical and Aerospace Engineering

MEA 589 Diffraction, Microscopy and Spectroscopy Techniques

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February 12, 2004

HOMEWORK NO. 4

SOLUTION

Problem 1

(a) The rock salt structure

The rock salt structure is based on the F cubic Bravais lattice, of which there are a number of unit cells. The most common unit cells are the cubic non-primitive unit cell and the rhombohedral primitive unit cell. Different unit cells correspond to different $\vec{a}_i$; so that the $\vec{b}_i$ are also different. As a result, $\vec{G}_m = \sum_i m_i \vec{b}_i$ also depends on the choice of unit cell. The structure factor, however, can be calculated by using any unit cell. In other words, the condition for constructive interference at a certain reciprocal lattice point $\vec{G}_m$ is independent of the choice of unit cell. The derivation of the structure factor of the rock salt structure is given below by first using the rhombohedral unit cell and then using the cubic unit cell.

Using the rhombohedral unit cell

The rhombohedral unit cell of the F cubic Bravais lattice is shown in Fig. 2.5 on p. 57 of the Notes. The fundamental translation vectors in direct and reciprocal space are given by

$$\vec{a}_1 = \frac{a}{2}(1,0,1) \qquad \vec{b}_1 = \frac{2\pi}{a}(1,\bar{1},1)$$

$$\vec{a}_2 = \frac{a}{2}(1,1,0) \qquad \vec{b}_2 = \frac{2\pi}{a}(1,1,\bar{1})$$

$$\vec{a}_3 = \frac{a}{2}(0,1,1) \qquad \vec{b}_3 = \frac{2\pi}{a}(\bar{1},1,1)$$

Hence,

$$\vec{G}_m = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$$

$$= \frac{2\pi}{a}\left(m_1 + m_2 - m_3,\ -m_1 + m_2 + m_3,\ m_1 - m_2 + m_3\right).$$

There are one cation and one anion per unit cell, since this unit cell has only one lattice point per unit cell. Let the lattice points per occupied by the cations. Then the $\vec{\rho}_j$'s are $(0,0,0)$ for the cation and $\frac{a}{2}(1,1,1)$ for the anion. Note that other choices of the anion position can be used in the basis.

The structure factor is

$$\underline{A}_s(-\vec{G}_m) = \sum_j \underline{S}_j\,\underline{A}\,e^{-i\vec{G}_m\cdot\vec{\rho}_j}$$

$$= \underline{A}\left[\underline{S}_c + \underline{S}_A\,e^{-i\pi(m_1+m_2+m_3)}\right],$$

where $\underline{S}_c$ and $\underline{S}_A$ are the scattering efficiencies for the cation and anion respectively.

If $(m_1 + m_2 + m_3)$ is even,

$$\underline{A}_s(-\vec{G}_m) = \underline{A}\ (\underline{S}_c + \underline{S}_A)$$

If $(m_1 + m_2 + m_3)$ is odd,

$$\underline{A}_s(-\vec{G}_m) = \underline{A}\ (\underline{S}_c - \underline{S}_A).$$

Thus, $\underline{A}_s(-\vec{G}_m)$ does not equal to zero for any $\vec{G}_m$. In other words, constructive interference occurs at all $\vec{G}_m$, where $\vec{G}_m$ are the reciprocal lattice vectors corresponding to the rhombohedral unit cell.

Since the intensity is proportional to $|\underline{A}_s(-\vec{G}_m)|^2$ diffraction lines corresponding to $\vec{G}_m$ such that $m_1 + m_2 + m_3$ is even are stronger than those corresponding to $\vec{G}_m$ such that $m_1 + m_2 + m_3$ is odd

Using the cubic unit cell

This non-primitive unit cell contains four lattice points per unit cell, so there are four cations and four anions per unit cell. Again let the cations occupy the lattice points. Thus the $\vec{f}_j$ are

cations: $(0,0,0)$, $\frac{a}{2}(1,1,0)$, $\frac{a}{2}(1,0,1)$, $\frac{a}{2}(0,1,1)$

anions: $\frac{a}{2}(1,1,1)$, $\frac{a}{2}(0,0,1)$, $\frac{a}{2}(0,1,0)$, $\frac{a}{2}(1,0,0)$.

The fundamental translation vectors are

$$\vec{a}_1 = a(1,0,0) \qquad \vec{b}_1 = \frac{2\pi}{a}(1,0,0)$$

$$\vec{a}_2 = a(0,1,0) \qquad \vec{b}_2 = \frac{2\pi}{a}(0,1,0)$$

$$\vec{a}_3 = a(0,0,1) \qquad \vec{b}_3 = \frac{2\pi}{a}(0,0,1)$$

Hence,

$$\vec{G}_m = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$$

$$= \frac{2\pi}{a}(m_1, m_2, m_3)$$

The structure factor is

$$\underline{A}_S(-\vec{G}_m) = \sum_j \underline{S}_j \underline{A}\, e^{-i\vec{G}_m\cdot\vec{\rho}_j}$$

$$= \underline{A}\left\{\underline{S}_C\left[1 + e^{-i\pi(m_1+m_2)} + e^{-i\pi(m_1+m_3)} + e^{-i\pi(m_2+m_3)}\right]\right.$$

$$\left. + \underline{S}_A\left[e^{-i\pi(m_1+m_2+m_3)} + e^{-i\pi m_3} + e^{-i\pi m_2} + e^{-i\pi m_1}\right]\right\}$$

$$\underline{A}_S(-\vec{G}_m) = \underline{A}\left\{\underline{S}_C\left[1 + e^{-i\pi(m_1+m_2)} + e^{-i\pi(m_1+m_3)} + e^{-i\pi(m_2+m_3)}\right]\right.$$

$$\left. + \underline{S}_A\, e^{-i\pi(m_1+m_2+m_3)}\left[1 + e^{i\pi(m_1+m_2)} + e^{i\pi(m_1+m_3)} + e^{i\pi(m_2+m_3)}\right]\right\}$$

Since

$$e^{n\pi i} = e^{-n\pi i}, \text{ where } n \text{ is any integer},$$

$$\underline{A}_s(-\vec{G}_m) = \underline{A}\left[\underline{S}_c + \underline{S}_A e^{-i\pi(m_1+m_2+m_3)}\right]\left[1+e^{-i\pi(m_1+m_2)}+e^{-i\pi(m_1+m_3)}+e^{-i\pi(m_2+m_3)}\right]$$

Note that the second term in brackets is merely the structure factor for the FCC structure; whereas the first term in brackets describes the basis which consists of a cation at $(0,0,0)$ and an anion at $\frac{a}{2}(1,1,1)$. (Other choices of the anion position can be used for the basis instead). The second term in brackets is non-zero only for unmixed indices (i.e., m_i all odd or all even)

For m_i all even,

$$\underline{A}_s(-\vec{G}_m) = 4\,\underline{A}\,(\underline{S}_c + \underline{S}_A).$$

For m_i all odd,

$$\underline{A}_s(-\vec{G}_m) = 4\,\underline{A}\,(\underline{S}_c - \underline{S}_A)$$

Wherever a crystal structure is an interpenetration of two substructures (as the rock salt structure is an interpenetration of two FCC substructures), the structure factor can be derived with much less algebra by factoring the common translations out of the structure factor expression and inserting the known values of the terms representing the translation from one substructure to the other.

(b) The diamond structure

The diamond structure is based on the F cubic Bravais lattice, with two atoms of the same element in the basis. The primitive unit cell is rhombohedral, with two atoms per unit cell. The cubic unit cell, on the other hand, has eight atoms per unit cell.

Using the rhombohedral unit cell

$$\vec{a}_1 = \frac{a}{2}(1,0,1) \qquad \vec{b}_1 = \frac{2\pi}{a}(1,\bar{1},1)$$

$$\vec{a}_2 = \frac{a}{2}(1,1,0) \qquad \vec{b}_2 = \frac{2\pi}{a}(1,1,\bar{1})$$

$$\vec{a}_3 = \frac{a}{2}(0,1,1) \qquad \vec{b}_3 = \frac{2\pi}{a}(\bar{1},1,1)$$

$$\vec{G}_m = \sum_i m_i \vec{b}_i = \frac{2\pi}{a}(m_1+m_2-m_3, -m_1+m_2+m_3, m_1-m_2+m_3)$$

$$\vec{\rho}_1 = (0,0,0), \quad \vec{\rho}_2 = \frac{a}{4}(1,1,1)$$

$$\underline{A}_S(-\vec{G}_m) = \sum_j \underline{S}_j \underline{A}\, e^{-i\vec{G}_m\cdot\vec{\rho}_j}$$

$$= \underline{A}\,\underline{S}\left[1 + e^{-i\frac{\pi}{2}(m_1+m_2+m_3)}\right]$$

If $m_1+m_2+m_3 = 4n$, where n = integer,

$$\underline{A}_S(-\vec{G}_m) = \underline{A}\,\underline{S}(1+1) = 2\,\underline{A}\,\underline{S}$$

If $m_1+m_2+m_3 = 2(2n+1)$, where n = integer,

$$\underline{A}_S(-\vec{G}_m) = \underline{A}\,\underline{S}(1-1) = 0$$

If $m_1 + m_2 + m_3 = 2n+1$, where n = integer.

$$\underline{A}_S(-\vec{G}_m) = \underline{A}\,\underline{S}\left(1 + e^{-i\frac{\pi}{2}n}\right) \neq 0$$

The condition for constructive interference is thus

$$m_1 + m_2 + m_3 \neq 2(2n+1), \text{ where } n = \text{integer}.$$

Using the cubic unit cell

$$\vec{a}_1 = a(1,0,0) \qquad \vec{b}_1 = \frac{2\pi}{a}(1,0,0)$$
$$\vec{a}_2 = a(0,1,0) \qquad \vec{b}_2 = \frac{2\pi}{a}(0,1,0)$$
$$\vec{a}_3 = a(0,0,1) \qquad \vec{b}_3 = \frac{2\pi}{a}(0,0,1)$$

$$\vec{G}_m = \sum_i m_i \vec{b}_i = \frac{2\pi}{a}(m_1, m_2, m_3)$$

$$\vec{\rho}_1 = (0,0,0), \qquad \vec{\rho}_5 = \frac{a}{4}(1,1,1)$$
$$\vec{\rho}_2 = \frac{a}{2}(1,1,0) \qquad \vec{\rho}_6 = \frac{a}{4}(3,3,1)$$
$$\vec{\rho}_3 = \frac{a}{2}(1,0,1) \qquad \vec{\rho}_7 = \frac{a}{4}(3,1,3)$$
$$\vec{\rho}_4 = \frac{a}{2}(0,1,1) \qquad \vec{\rho}_8 = \frac{a}{4}(1,3,3)$$

$$\underline{A}_S(-\vec{G}_m) = \sum_j \underline{S}_j \underline{A}\, e^{-i\vec{G}_m \cdot \vec{\rho}_j}$$

$$= \underline{S}\,\underline{A}\left\{1 + e^{-i\pi(m_1+m_2)} + e^{-i\pi(m_1+m_3)} + e^{-i\pi(m_2+m_3)}\right.$$
$$\left. + e^{-i\frac{\pi}{2}(m_1+m_2+m_3)}\left[1 + e^{-i\pi(m_1+m_2)} + e^{-i\pi(m_1+m_3)} + e^{-i\pi(m_2+m_3)}\right]\right\}$$

$$= \underline{S}\,\underline{A}\left[1 + e^{-i\frac{\pi}{2}(m_1+m_2+m_3)}\right]\cdot\left[1 + e^{-i\pi(m_1+m_2)} + e^{-i\pi(m_1+m_3)} + e^{-i\pi(m_2+m_3)}\right]$$

$\underline{A}_s(-\vec{G}_m) = 0$ when $m_1 + m_2 + m_3 = 2(2n+1)$, where n = integer

or

when m_1, m_2, m_3 are mixed (i.e. not all even and not all odd).

Otherwise, $\underline{A}_s(-\vec{G}_m) \neq 0$.

In particular,

when $m_1 + m_2 + m_3 = 4n$ (where n = integer) and m_1, m_2, m_3 all even,

$$\underline{A}_s(-\vec{G}_m) = \underline{S}\,\underline{A}(2)(4) = 8\,\underline{S}\,\underline{A};$$

when m_1, m_2, m_3 all odd,

$$\underline{A}_s(-\vec{G}_m) = \underline{S}\,\underline{A}\left[1 + e^{-i\frac{\pi}{2}(m_1+m_2+m_3)}\right](4) \neq 0.$$

Therefore, the condition for constructive interference is

m_1, m_2, m_3 all odd

or

m_1, m_2, m_3 all even and $m_1 + m_2 + m_3 = 4n$

(c) The zinc blende structure

The zinc blende structure is the same as the diamond structure except that the two atoms in the basis are of different elements.

Using the rhombohedral unit cell

$$\underline{A}_s(-\vec{G}_m) = \underline{A}\left[\underline{S}_1 + \underline{S}_2 e^{-i\frac{\pi}{2}(m_1+m_2+m_3)}\right]$$

If $m_1 + m_2 + m_3 = 4n$, where n = integer,

$$\underline{A}_S(-\vec{G}_m) = \underline{A}\,(\underline{S}_1 + \underline{S}_2) \neq 0$$

If $m_1 + m_2 + m_3 = 2(2n+1)$, where n = integer,

$$\underline{A}_S(-\vec{G}_m) = \underline{A}\,(\underline{S}_1 - \underline{S}_2) \neq 0, \quad \text{unless } \underline{S}_1 = \underline{S}_2$$

If $m_1 + m_2 + m_3 = 2n+1$, where n = integer,

$$\underline{A}_S(-\vec{G}_m) = \underline{A}\,(\underline{S}_1 + \underline{S}_2 e^{-i\frac{\pi}{2}n}) \neq 0$$

The condition for constructive interference is thus dependent on the relation between $\underline{S}_1$ and $\underline{S}_2$. If $\underline{S}_1 = \underline{S}_2$, $\underline{A}_S(-\vec{G}_m) = 0$ when $m_1 + m_2 + m_3 = 2(2n+1)$, where n = integer. Otherwise, $\underline{A}_S(-\vec{G}_m)$ does not vanish for any $\vec{G}_m$.

Using the cubic unit cell

$$\underline{A}_S(-\vec{G}_m) = \underline{A}\left[\underline{S}_1 + \underline{S}_2 e^{-i\frac{\pi}{2}(m_1+m_2+m_3)}\right]\cdot\left[1 + e^{-i\pi(m_1+m_2)} + e^{-i\pi(m_1+m_3)} + e^{-i\pi(m_2+m_3)}\right]$$

$= 0$ where m_1, m_2, m_3 are mixed.

The condition for constructive interference is

m_1, m_2, m_3 all odd.

or

m_1, m_2, m_3 all even and $m_1 + m_2 + m_3 = 4n$ (n = integer)

Problem 2

$$\lambda = 2d \sin\theta$$

Hence, $$d = \frac{\lambda}{2 \sin\theta}$$

$$2\theta = 44.4^\circ, \text{ or } \theta = 22.2^\circ$$

$$\lambda = 1.54\ \text{Å}$$

Hence,

$$d = \frac{1.54\ \text{Å}}{2 \sin(22.2^\circ)} = 2.04\ \text{Å}$$

Since $$\frac{1}{d^2} = \frac{h^2 + k^2 + \ell^2}{a^2}$$,

for the (110) planes,

$$\frac{1}{d^2} = \frac{1^2 + 1^2 + 0^2}{a^2} = \frac{2}{a^2}$$

Thus,

$$a = \sqrt{2}\, d = \sqrt{2}\,(2.04\ \text{Å}) = \underline{\underline{2.88\ \text{Å}}}$$

Problem 3

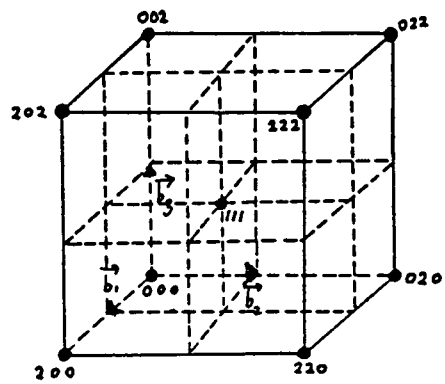
The reciprocal lattice of FCC forms an I cubic Bravais lattice, as shown below. Using the non-primitive cubic unit cell for the FCC structure, the structure factor is given by

$$\underline{A}_s(-\vec{G}_m) = A \sum \left[1 + e^{-i\pi(m_1+m_2)} + e^{-i\pi(m_1+m_3)} + e^{-i\pi(m_2+m_3)}\right],$$

where $$\vec{G}_m = \sum_i m_i \vec{b}_i = \frac{2\pi}{a}(m_1, m_2, m_3).$$

The structure factor was obtained by noting that the positions of the four atoms in the basis are

$$\vec{\rho}_1 = (0, 0, 0)$$
$$\vec{\rho}_2 = \frac{a}{2}(1, 1, 0)$$
$$\vec{\rho}_3 = \frac{a}{2}(1, 0, 1)$$
$$\vec{\rho}_4 = \frac{a}{2}(0, 1, 1)$$



Reciprocal lattice of the FCC Structure

$A_s(-\vec{G}_m) = 0$ when m_1, m_2 and m_3 are mixed (i.e. not all odd or all even).
Thus, $\vec{G}_m$'s with $A_s(-\vec{G}_m) \neq 0$ are

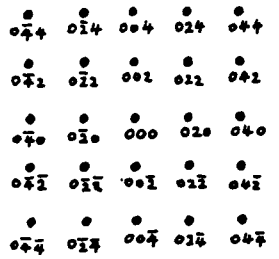
m_1	m_2	m_3
1	1	1
2	0	0
2	2	0
3	1	1
2	2	2
4	0	0
3	3	1
4	2	0

etc.

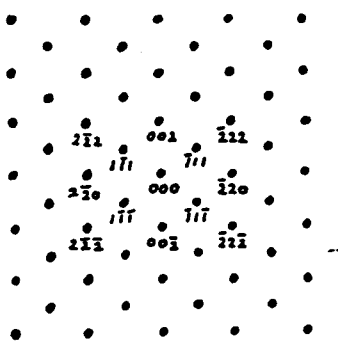
In the above list, $\vec{G}_m$'s with the same $|\vec{G}_m|$ are not shown.

In electron diffraction, the Ewald sphere is so large that a reciprocal lattice plane rather than just a reciprocal lattice point satisfies the Laue diffraction condition. Therefore an electron diffraction pattern shows a certain reciprocal lattice plane.

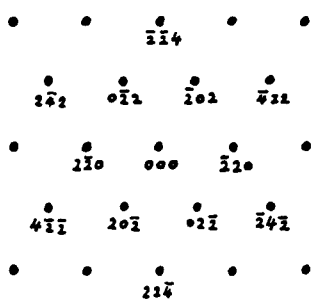
(a) (100)



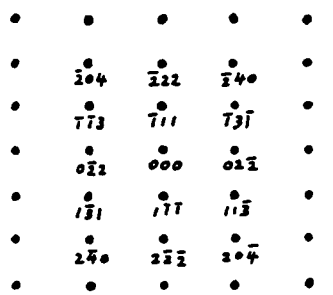
(b) (110)



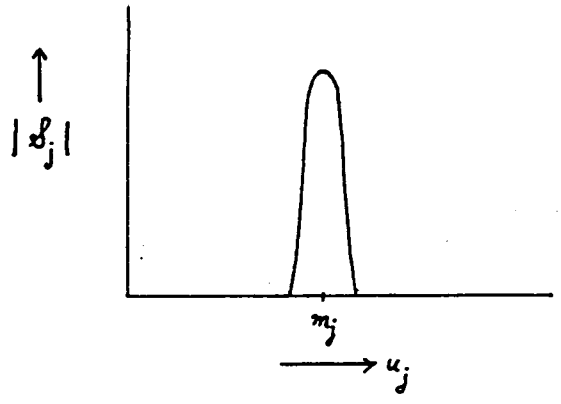
(c) (111)

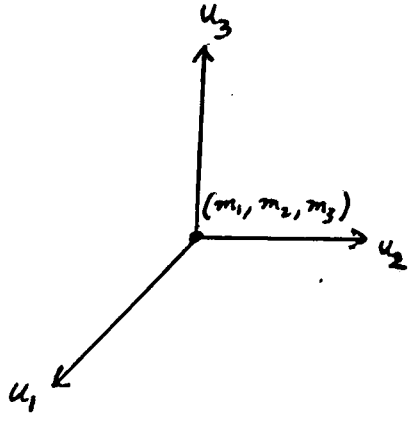


(d) (211)



Problem 4





$\vec{K}$ space

$\vec{K} \equiv u_1\vec{b}_1 + u_2\vec{b}_2 + u_3\vec{b}_3$

$$\mathcal{S} = \mathcal{S}_1\mathcal{S}_2\mathcal{S}_3 = e^{-\pi i[u_1(N_1+1)+u_2(N_2+1)+u_3(N_3+1)]} \frac{\sin \pi u_1 N_1}{\sin \pi u_1} \frac{\sin \pi u_2 N_2}{\sin \pi u_2} \frac{\sin \pi u_3 N_3}{\sin \pi u_3}$$

$$|\mathcal{S}| = \frac{\sin \pi u_1 N_1}{\sin \pi u_1} \frac{\sin \pi u_2 N_2}{\sin \pi u_2} \frac{\sin \pi u_3 N_3}{\sin \pi u_3} = 0 \quad \text{when either} \quad u_1 = m_1 + \frac{\text{integer}}{N_1},$$

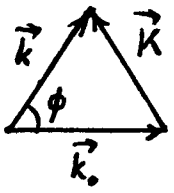
or $u_2 = m_2 + \frac{\text{integer}}{N_2}$, or $u_3 = m_3 + \frac{\text{integer}}{N_3}$.

Consider the values of u_j closest to m_j that give $|\mathcal{S}| = 0$, since we want to obtain the width of the peak. Thus, $|\mathcal{S}| = 0$ when either $u_1 = m_1 + \frac{1}{N_1}$, or $u_2 = m_2 + \frac{1}{N_2}$, or $u_3 = m_3 + \frac{1}{N_3}$.

(a) Let $u_1 = m_1 + \frac{1}{N_1}$, $u_2 = m_2$, $u_3 = m_3$. Then

$$\vec{K} = \left(m_1 + \frac{1}{N_1}\right)\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$$

In $\vec{K}$ space, the extent of the peak along $\vec{b}_1$ is from $\left(m_1 - \frac{1}{N_1}\right)\vec{b}_1$ to $\left(m_1 + \frac{1}{N_1}\right)\vec{b}_1$. If N_1 is small, the peak occurs over a longer region along $\vec{b}_1$.



$$|\vec{K}| = \frac{4\pi}{\lambda}\sin\frac{\phi}{2}$$

For $\vec{K} = \left(m_1 + \frac{1}{N_1}\right)\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$, let the corresponding ϕ be ϕ_1

$$\sin\frac{\phi_1}{2} = \frac{\lambda}{4\pi}|\vec{K}| = \frac{\lambda}{4\pi}\left|\left(m_1+\frac{1}{N_1}\right)\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3\right|$$

For the cubic system, $\vec{b}_1 = \frac{2\pi}{a}(1,0,0)$, $\vec{b}_2 = \frac{2\pi}{a}(0,1,0)$, $\vec{b}_3 = \frac{2\pi}{a}(0,0,1)$. Then

$$\sin\frac{\phi_1}{2} = \frac{\lambda}{4\pi}\frac{2\pi}{a}\left[\left(m_1+\frac{1}{N_1}\right)^2 + m_2^2 + m_3^2\right]^{1/2}$$

(b) Let $u_1 = m_1$, $u_2 = m_2 + \frac{1}{N_2}$, $u_3 = m_3$. Then

$$\vec{K} = m_1\vec{b}_1 + \left(m_2 + \frac{1}{N_2}\right)\vec{b}_2 + m_3\vec{b}_3$$

$$\sin\frac{\phi_2}{2} = \frac{\lambda}{4\pi}\left|\, m_1\vec{b}_1 + \left(m_2+\frac{1}{N_2}\right)\vec{b}_2 + m_3\vec{b}_3\,\right|$$

$$= \frac{\lambda}{4\pi}\frac{2\pi}{a}\left[m_1^2 + \left(m_2+\frac{1}{N_2}\right)^2 + m_3^2\right]^{1/2} \quad \text{(For cubic system)}$$

(c) Let $u_1 = m_1$, $u_2 = m_2$, $u_3 = m_3 + \frac{1}{N_3}$. Then

$$\vec{K} = m_1\vec{b}_1 + m_2\vec{b}_2 + \left(m_3 + \frac{1}{N_3}\right)\vec{b}_3$$

$$\sin\frac{\phi_3}{2} = \frac{\lambda}{4\pi}\left|\, m_1\vec{b}_1 + m_2\vec{b}_2 + \left(m_3+\frac{1}{N_3}\right)\vec{b}_3\,\right|$$

$$= \frac{\lambda}{4\pi}\frac{2\pi}{a}\left[m_1^2 + m_2^2 + \left(m_3+\frac{1}{N_3}\right)^2\right]^{1/2} \quad \text{(For cubic system)}$$

Note: If $N_1 \ll N_2 \sim N_3$, the peak is streaked along $\vec{b}_1$.
If $N_2 \ll N_1 \sim N_3$, the peak is streaked along $\vec{b}_2$.
If $N_3 \ll N_1 \sim N_2$, the peak is streaked along $\vec{b}_3$.

$|\mathcal{S}| = N_1 N_2 N_3$ when $u_1 = m_1$, $u_2 = m_2$, $u_3 = m_3$. Then
$\vec{K} = \vec{G}_m = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$. The corresponding $\frac{\phi}{2} = \theta_B$.

$$\sin\theta_B = \frac{\lambda}{4\pi}|\vec{G}_m| = \frac{\lambda}{4\pi}\frac{2\pi}{a}(m_1^2+m_2^2+m_3^2)^{1/2} \quad \text{(For cubic system)}$$

The value of $\frac{\phi_1}{2}$, $\frac{\phi_2}{2}$ or $\frac{\phi_3}{2}$ that is closest to θ_B is the value of θ_1 (θ_1 is the value of θ where the intensity first hits zero).

Suppose $\frac{\phi_1}{2}$ is closest to θ_B. Then

$$2(\theta_1-\theta_B) = 2\left(\frac{\phi_1}{2}-\theta_B\right) = 2\left\{\sin^{-1}\frac{\lambda}{2a}\left[\left(m_1+\frac{1}{N_1}\right)^2+m_2^2+m_3^2\right]^{1/2} - \sin^{-1}\frac{\lambda}{2a}(m_1^2+m_2^2+m_3^2)^{1/2}\right\}$$

$$= 2\left\{\sin^{-1}\frac{\lambda}{2a}\left(m_1^2+m_2^2+m_3^2+2\frac{m_1}{N_1}+\frac{1}{N_1^2}\right)^{1/2} - \sin^{-1}\frac{\lambda}{2a}(m_1^2+m_2^2+m_3^2)^{1/2}\right\}$$

Note: $\theta_B\uparrow$ $d\downarrow$ $|\vec{G}_m|\uparrow$ $m_i\uparrow$ $(\theta_1-\theta_B)\uparrow$ $B\uparrow$

Problem 5

$$eV_{min} = h\nu_{min} = \frac{hc}{\lambda_{max}}$$

$$\lambda = 2d\sin\theta \Rightarrow \lambda_{max} = 2d_{max}$$

$$d_{max} = \frac{2\pi}{|\vec{G}_m|_{min}}$$

For the FCC structure, $\vec{G}_m = \frac{2\pi}{a}(1,1,1)$ corresponds to $|\vec{G}_m|_{min}$.
Thus,

$$|\vec{G}_m|_{min} = \frac{2\pi}{a}\sqrt{3}.$$

Hence,

$$V_{min} = \frac{hc}{e\lambda_{max}} = \frac{hc}{e\,2d_{max}} = \frac{hc}{e\,2\frac{2\pi}{|\vec{G}_m|_{min}}} = \frac{hc}{e\,2\frac{2\pi}{\frac{2\pi}{a}\sqrt{3}}} = \frac{\sqrt{3}\,hc}{2ea}$$

$$= \frac{\sqrt{3}(6.626\times10^{-34})(2.998\times10^{8})}{2(1.602\times10^{-19})(4.05\times10^{-10})} = 2651\ V = \underline{\underline{2.65\ kV}}$$

Problem 6

For all "simple" crystal structures (simple cubic, simple tetragonal, simple rhombohedral, etc.), the conventional unit cells are the primitive unit cells. By using the primitive unit cell with only one atom in the basis, the structure factor $A_S(-\vec{G}_m)$ does not vanish for any $\vec{G}_m$. Therefore, there are diffraction lines corresponding to all combinations of m_1, m_2 and m_3. Since

$$\frac{\lambda}{2 \sin\theta} = d = \frac{2\pi}{|\vec{G}_m|} ,$$

the diffraction angle 2θ depends on the magnitude of $\vec{G}_m$ only. Thus all reflections corresponding to different $\vec{G}_m$'s of the same magnitude occur at the same 2θ angle.

$$\vec{a}_1 = a(1,0,0) \qquad \vec{b}_1 = \frac{2\pi}{a}(1,0,0)$$

$$\vec{a}_2 = a(0,1,0) \qquad \vec{b}_2 = \frac{2\pi}{a}(0,1,0)$$

$$\vec{a}_3 = a(0,0,1) \qquad \vec{b}_3 = \frac{2\pi}{a}(0,0,1)$$

$$\therefore \vec{G}_m = \sum_i m_i \vec{b}_i = \frac{2\pi}{a}(m_1, m_2, m_3)$$

$$|\vec{G}_m| = \frac{2\pi}{a}\sqrt{m_1^2 + m_2^2 + m_3^2}$$

Thus, reflections corresponding to the following $\vec{G}_m$'s occur at the same 2θ angle:

m_1	m_2	m_3
1	0	0
0	1	0
0	0	1
-1	0	0
0	-1	0
0	0	-1

For all these six $\vec{G}_m$'s, $|\vec{G}_m| = \frac{2\pi}{a}$. This diffraction line is referred to as the "100 line."

Therefore, representative $\vec{G}_m$'s for the three diffraction lines of the lowest 2θ angles are

m_1	m_2	m_3
1	0	0
1	1	0
1	1	1

For the 100 line, $|\vec{G}_m| = \frac{2\pi}{a}$. Hence, $d = \frac{2\pi}{|\vec{G}_m|} = a = 3.00\,\text{Å}$

$$\sin\theta = \frac{\lambda}{2d}$$

From Appendix 7 on p. 509 of Cullity, for a Cu target,

$$\lambda_{K\alpha_1} = 1.540562\,\text{Å}$$

$$\lambda_{K\alpha_2} = 1.544390\,\text{Å}$$

The wavelength of the unresolved Kα doublet is usually taken as the weighted average of the wavelengths of its components, $K\alpha_1$ being given twice the weight of $K\alpha_2$, since it is twice as strong. Thus the wavelength of the unresolved Cu Kα line is

$$\frac{1}{3}(2 \times 1.540562 + 1.544390)\ \text{Å} = 1.5418\ \text{Å}$$

Thus, for the 100 line,

$$\sin\theta = \frac{\lambda}{2d} = \frac{1.5418\ \text{Å}}{2(3.00\ \text{Å})} = 0.25696$$

or

$$\theta = 14.896^\circ$$

or

$$2\theta = \underline{\underline{29.79^\circ}}$$

For the 110 line, $|\vec{G}_m| = \frac{2\pi}{a}\sqrt{1^2+1^2+0^2} = \frac{2\pi}{a}\sqrt{2}$.
Hence,

$$d = \frac{2\pi}{|\vec{G}_m|} = \frac{a}{\sqrt{2}} = \frac{3.00\ \text{Å}}{\sqrt{2}} = 2.1216\ \text{Å}$$

$$\sin\theta = \frac{\lambda}{2d} = \frac{1.5418\ \text{Å}}{2(2.1216\ \text{Å})} = 0.36335$$

$$\theta = 21.314^\circ$$

$$2\theta = \underline{\underline{42.63^\circ}}$$

For the 111 line, $|\vec{G}_m| = \frac{2\pi}{a}\sqrt{1^2+1^2+1^2} = \frac{2\pi}{a}\sqrt{3}$

Hence,

$$d = \frac{2\pi}{|\vec{G}_m|} = \frac{a}{\sqrt{3}} = \frac{3.00\,\text{Å}}{\sqrt{3}} = 1.732\,\text{Å}$$

$$\sin\theta = \frac{\lambda}{2d} = \frac{1.5418\,\text{Å}}{2(1.732\,\text{Å})} = 0.44509$$

$$\theta = 26.413^\circ$$

$$2\theta = \underline{\underline{52.83^\circ}}$$

Therefore the three lowest angle lines occur at $2\theta = 29.79^\circ$, 42.63° and 52.83°.

(b) Simple tetragonal ($c > a$)

$$\vec{a}_1 = a(1,0,0) \qquad \vec{b}_1 = \frac{2\pi}{a}(1,0,0)$$
$$\vec{a}_2 = a(0,1,0) \qquad \vec{b}_2 = \frac{2\pi}{a}(0,1,0)$$
$$\vec{a}_3 = c(0,0,1) \qquad \vec{b}_3 = \frac{2\pi}{c}(0,0,1)$$

$$\vec{G}_m = \sum_i m_i \vec{b}_i = \left(\frac{2\pi}{a}m_1, \frac{2\pi}{a}m_2, \frac{2\pi}{c}m_3\right)$$

$$|\vec{G}_m| = 2\pi\left[\left(\frac{m_1}{a}\right)^2 + \left(\frac{m_2}{a}\right)^2 + \left(\frac{m_3}{c}\right)^2\right]^{\frac{1}{2}}$$

Representative $\vec{G}_m$'s for the three diffraction lines of the lowest 2θ angles are

m_1	m_2	m_3
0	0	1
1	0	0
1	0	1

Note that $|\vec{G}_m|$ is the same for 1 0 0 and 0 1 0, but is different for 0 0 1. Moreover, $|\vec{G}_m|$ for 0 0 1 is smaller than that for 1 0 0 because $|\vec{b}_3| < |\vec{b}_2|$ ($c > a$). For the same reason, $|\vec{G}_m|$ for 1 0 1 is smaller than that for 1 1 0.

For the 0 0 1 line, $|\vec{G}_m| = \frac{2\pi}{c}$.

Hence,

$$d = \frac{2\pi}{|\vec{G}_m|} = c = 3.00 \text{ Å}$$

$$\sin\theta = \frac{\lambda}{2d} = \frac{1.5418 \text{ Å}}{2(3.00 \text{ Å})} = 0.25696$$

$$\theta = 14.896^\circ$$

$$2\theta = \underline{\underline{29.79^\circ}}$$

For the 100 line, $|\vec{G}_m| = \frac{2\pi}{a}$

Hence,

$$d = \frac{2\pi}{|\vec{G}_m|} = a = 2.00\ \text{Å}$$

$$\sin\theta = \frac{\lambda}{2d} = \frac{1.5418\ \text{Å}}{2(2.00\ \text{Å})} = 0.38545$$

$$\theta = 22.689^\circ$$

$$2\theta = \underline{\underline{45.38^\circ}}$$

For the 101 line, $|\vec{G}_m| = 2\pi\left(\frac{1}{a^2} + \frac{1}{c^2}\right)^{1/2}$

Hence,

$$d = \frac{2\pi}{|\vec{G}_m|} = \left(\frac{1}{a^2} + \frac{1}{c^2}\right)^{-1/2} = 1.6642\ \text{Å}$$

$$\sin\theta = \frac{\lambda}{2d} = \frac{1.5418\ \text{Å}}{2(1.6642\ \text{Å})} = 0.46322$$

$$\theta = 27.616^\circ$$

$$2\theta = \underline{\underline{55.23^\circ}}$$

Therefore the three lowest angle lines occur at 2θ of 29.79°, 45.38° and 55.23°.

(c) Simple tetragonal ($c < a$)

With $c < a$, the representative $\vec{G}_m$'s for the three diffraction lines of the lowest 2θ angles are

m_1	m_2	m_3
1	0	0
1	1	0
0	0	1

Whether $|\vec{G}_m|$ is larger for 001 or 110 depends on the c/a ratio.

For the 100 line, $|\vec{G}_m| = \frac{2\pi}{a}$

Hence,

$$d = \frac{2\pi}{|\vec{G}_m|} = a = 3.00\ \text{Å}$$

$$\sin\theta = \frac{\lambda}{2d} = \frac{1.5418\ \text{Å}}{2(3.00\ \text{Å})} = 0.25696$$

$$2\theta = \underline{\underline{29.79^\circ}}$$

For the 110 line, $|\vec{G}_m| = \frac{2\pi}{a}\sqrt{1^2+1^2} = \frac{2\pi}{a}\sqrt{2}$

Hence,

$$d = \frac{2\pi}{|\vec{G}_m|} = \frac{a}{\sqrt{2}} = \frac{3.00\ \text{Å}}{\sqrt{2}} = 2.1216\ \text{Å}$$

$$\sin\theta = \frac{\lambda}{2d} = \frac{1.5418\ \text{Å}}{2(2.1216\ \text{Å})} = 0.36335$$

$$\theta = 21.314^\circ$$

$$2\theta = \underline{\underline{42.63^\circ}}$$

For the 001 line, $|\vec{G}_m| = \frac{2\pi}{c}$.
Hence,

$$d = \frac{2\pi}{|\vec{G}_m|} = c = 2.00\ \text{Å}$$

$$\sin\theta = \frac{\lambda}{2d} = \frac{1.5418\ \text{Å}}{2(2.00\ \text{Å})} = 0.38545$$

$$\theta = 22.689^\circ$$

$$2\theta = \underline{\underline{45.38^\circ}}$$

The value of 2θ is slightly higher for the 001 line than for the 110 line. This is true for the c/a value encountered in this problem.
The three lowest angle lines occur at 2θ = 29.79°, 42.63° and 45.38°.