Solutions for Homework 2

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1 Interplanar separation

Suppose the plane intercepts x,y,z axes at $x_1\overrightarrow{a_1}, x_2\overrightarrow{a_2}, x_3\overrightarrow{a_3}$ respectively. Then $x_1 : x_2 : x_3 = \frac{1}{h} : \frac{1}{k} : \frac{1}{l}$.

(a) Prove that the reciprocal lattice vector $\overrightarrow{G} = h\overrightarrow{b_1} + k\overrightarrow{b_2} + l\overrightarrow{b_3}$ is perpendicular to this plane.

Two vectors in the plane are $(x_2\overrightarrow{a_2} - x_1\overrightarrow{a_1})$ and $(x_3\overrightarrow{a_3} - x_1\overrightarrow{a_1})$ Thus the normal vector to the plane is

$$(x_2\overrightarrow{a_2} - x_1\overrightarrow{a_1}) \times (x_3\overrightarrow{a_3} - x_1\overrightarrow{a_1})$$

$$= x_1x_3\overrightarrow{a_3} \times \overrightarrow{a_1} + x_1x_2\overrightarrow{a_1} \times \overrightarrow{a_2} + x_2x_3\overrightarrow{a_2} \times \overrightarrow{a_3}$$

$$= x_1x_2x_3(\frac{1}{x_1}\overrightarrow{a_2} \times \overrightarrow{a_3} + \frac{1}{x_2}\overrightarrow{a_3} \times \overrightarrow{a_1} + \frac{1}{x_3}\overrightarrow{a_1} \times \overrightarrow{a_2})$$

$$\sim h\overrightarrow{b_1} + k\overrightarrow{b_2} + l\overrightarrow{b_3}$$

Therefore $\overrightarrow{G} = h\overrightarrow{b_1} + k\overrightarrow{b_2} + l\overrightarrow{b_3}$ is perpendicular to this plane.

(b) Prove that the distance between two adjacent parallel planes of the lattice is $d(hkl) = \frac{2\pi}{\|G\|}$.

For any $\overrightarrow{R} = x_1\overrightarrow{a_1} + x_2\overrightarrow{a_2} + x_3\overrightarrow{a_3}$, the expression $e^{i\overrightarrow{G}\overrightarrow{R}} = const$. Since the lattice contain $0\overrightarrow{a_1}+0\overrightarrow{a_2}+0\overrightarrow{a_3}$, we obtain that $e^{i\overrightarrow{G}\overrightarrow{R}} = const = 1$. Therefore $\overrightarrow{G}\overrightarrow{R} = 2\pi n \Rightarrow \overrightarrow{G}\Delta\overrightarrow{R} = 2\pi\Delta n$.

The distance between two adjacent parallel plane ($\Delta n = 1$) is

$$d = \frac{\overrightarrow{G}}{\|\overrightarrow{G}\|}\Delta\overrightarrow{R} = \frac{2\pi}{\|\overrightarrow{G}\|}$$

(c) For a simple cubic lattice,

$$\overrightarrow{G} = h\overrightarrow{b_1} + k\overrightarrow{b_2} + l\overrightarrow{b_3}$$

$$\|\overrightarrow{G}\| = \sqrt{h^2 + k^2 + l^2} \times (\frac{2\pi}{a})$$

Thus

$$d = \frac{2\pi}{\|G\|} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

.

2 Volume of Brillouin zone

According to the hint, the volume of a Brillouin zone is equal to the volume of the primitive parallelepiped in Fourier space. And the parallelepiped is described by

$$\vec{b_1} = 2\pi \frac{\vec{a_2} \times \vec{a_3}}{\vec{a_1} \cdot \vec{a_2} \times \vec{a_3}}$$

$$\vec{b_2} = 2\pi \frac{\vec{a_3} \times \vec{a_1}}{\vec{a_1} \cdot \vec{a_2} \times \vec{a_3}}$$

$$\vec{b_3} = 2\pi \frac{\vec{a_1} \times \vec{a_2}}{\vec{a_1} \cdot \vec{a_2} \times \vec{a_3}}$$

So the volume of the first Brillouin zone $V_{BZ} = \vec{b_1} \cdot \vec{b_2} \times \vec{b_3}$ and $V_c = \vec{a_1} \cdot \vec{a_2} \times \vec{a_3}$.

$$V_{BZ} = \frac{(2\pi)^3}{V_c^3} \vec{a_2} \times \vec{a_3} \cdot (\vec{a_3} \times \vec{a_1}) \times (\vec{a_1} \times \vec{a_2})$$

$$= \frac{(2\pi)^3}{V_c^3} \vec{a_2} \times \vec{a_3} \cdot (\vec{a_3} \cdot \vec{a_1} \times \vec{a_2}) \vec{a_1}$$

$$= \frac{(2\pi)^3}{V_c^3} (\vec{a_1} \cdot \vec{a_2} \times \vec{a_3})^2 = \frac{(2\pi)^3}{V_c}$$

3 With of diffraction maximum

$$F = \frac{1 - e^{-iM(a\Delta k)}}{1 - e^{-i(a\Delta k)}}$$

(a)

$$|F|^2 = F^* F = \frac{1 - e^{iM(a\Delta k)}}{1 - e^{i(a\Delta k)}} \frac{1 - e^{-iM(a\Delta k)}}{1 - e^{-i(a\Delta k)}}$$

$$= \frac{2 - e^{iM(a\Delta k)} - e^{-iM(a\Delta k)}}{2 - e^{i(a\Delta k)} - e^{-i(a\Delta k)}} = \frac{1 - \cos M(a \cdot \Delta k)}{1 - \cos a \cdot \Delta k}$$

$$= \frac{\sin^2 \frac{1}{2} M(a \cdot \Delta k)}{\sin^2 \frac{1}{2}(a \cdot \Delta k)}$$

where we've used $\cos\theta = 1 - 2\sin^2 \frac{\theta}{2}$.

(b)

$$a \cdot \Delta k = 2\pi h + \epsilon$$

$$|F|^2 = \frac{\sin^2(M\pi h + \frac{\epsilon}{2} M)}{\sin^2(\pi h + \frac{\epsilon}{2})} = \frac{\sin^2(\frac{M}{2}\epsilon)}{\sin^2(\frac{1}{2}\epsilon)}$$

For the first zero, $\frac{M}{2}\epsilon = \pi$, i.e, $\epsilon = \frac{2\pi}{M}$. So the width of the diffraction maximum is proportion to $1/M$.

4 Problem 4

We can read off the angles 2θ from Fig 17, and also from problem 1, we know

$$d(111) = \frac{a}{\sqrt{3}}, d(200) = \frac{a}{2}, d(220) = \frac{a}{2\sqrt{2}}$$

.

For lattice plane (111), $2\theta = 23.5^0$, plane (200), $2\theta = 27.3^0$,and plane (220), $2\theta = 38.5^0$.

So we can calculate the quantities $n\lambda = 2d\sin\theta$.

$$(111), \lambda = 0.235a$$

$$(200), \lambda = 0.236a$$

$$(220), \lambda = 0.233a$$

Thus, we can infer that $\lambda \simeq 0.235a$, which a is the lattice constant of the simple cubic.

The energy of the x-ray is then

$$E = \hbar\omega = \frac{hc}{\lambda} = \frac{hc}{0.235a}$$

If a is measured in the unit of $\dot{A}$, then

$$E = \frac{2\pi \cdot 0.6582 \times 10^{-15} eV \cdot sec \cdot 3 \times 10^8 \times 10^{10} \dot{A}/sec}{0.235a(\dot{A}} = \frac{5.279 \times 10^4}{a} eV$$

5 Problem 5

From Problem 1, we know $d = \frac{2\pi}{|\vec{G}|}$. Thus the Bragg condition $n\lambda = 2d\sin\theta$ can be cast into

$$\frac{4\pi}{|\vec{G}|}\sin\theta = n\lambda \Rightarrow \sin\theta = \frac{n\lambda}{4\pi}|h\vec{b_1} + k\vec{b_2} + l\vec{b_3}|$$

h,k,l integers.

For bcc,

$$\vec{b_1} = \frac{2\pi}{a}(\hat{y} + \hat{z}), \vec{b_2} = \frac{2\pi}{a}(\hat{z} + \hat{x}), \vec{b_3} = \frac{2\pi}{a}(\hat{x} + \hat{y})$$

$$\vec{G} = \frac{2\pi}{a}[(k+l)\hat{x} + (l+h)\hat{y} + (h+k)\hat{z}]$$

$$\Rightarrow |\vec{G}| = \frac{2\pi}{a}[(k+l)^2 + (l+h)^2 + (h+k)^2]^{1/2}$$

So the first few $|\vec{G}|$ can be

- $$|\vec{G}| = \frac{2\pi}{a}\sqrt{2}$$
  corresponding to$(h,k,l) = \pm(1,0,0), \pm(0,1,0), \pm(0,0,1)$

- $$|\vec{G}| = \frac{2\pi}{a}2$$
  corresponding to$(h,k,l) = \pm(2,-2,0), \pm(0,2,-2), \pm(-2,0,2)$

- $$|\vec{G}| = \frac{2\pi}{a}\sqrt{6}$$
  corresponding to$(h,k,l) = \pm(1,1,0), \pm(0,1,1), \pm(1,0,1), \pm(2,-1,-1), \pm(-1,2,-1), \pm(-1,-1,2)$

So $\sin\theta_1 : \sin\theta_2 : \sin\theta_3 = \sqrt{2} : 2 : \sqrt{6} \simeq 1 : 1.414 : 1.732$ for bcc.

For fcc,

$$\vec{b_1} = \frac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z}), \vec{b_2} = \frac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z}), \vec{b_3} = \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z})$$

$$\vec{G} = \frac{2\pi}{a}[(k+l-h)\hat{x} + (l+h-k)\hat{y} + (h+k-l)\hat{z}]$$

$$\Rightarrow |\vec{G}| = \frac{2\pi}{a}[(k+l-h)^2 + (l+h-k)^2 + (h+k-l)^2]^{1/2}$$

So the first few $|\vec{G}|$ can be

- $$|\vec{G}| = \frac{2\pi}{a}\sqrt{3}$$
  corresponding to$(h,k,l) = \pm(1,1,1), \pm(1,0,0), \pm(0,1,0), \pm(0,0,1)$

- $$|\vec{G}| = \frac{2\pi}{a}2$$
  corresponding to$(h,k,l) = \pm(1,0,1), \pm(0,1,1), \pm(1,1,0)$

- $$|\vec{G}| = \frac{2\pi}{a}\sqrt{8}$$
  corresponding to$(h,k,l) = \pm(1,1,2), \pm(2,1,1), \pm(1,2,1), \pm(1,0,-1), \pm(0,1,-1), \pm(1,-1,0)$

So $\sin\theta_1 : \sin\theta_2 : \sin\theta_3 = \sqrt{3} : 2 : \sqrt{8} \simeq 1 : 1.155 : 1.633$for fcc.
From the figure, we have

$$\sin\theta_1 : \sin\theta_2 : \sin\theta_3 = \sin\frac{23.5^0}{2} : \sin\frac{27.3^0}{2} : \sin\frac{38.5^0}{2}$$
$$= 1 : 1.159 : 1.619$$

which is much closer to the result of fcc than to that of bcc.

6 Structure factor of diamond

Here we give two ways to derive the result. The first is the long proof that follows the suggestion to consider diamond as simple cubic with 8 atoms per cell. The second is the short proof that uses the fact that diamond is fcc with 2 atoms per cell.

Diamond described as simple cubic with 8 atoms/cell:

The diamond structure can be described as a simple cubic lattice with the eight point basis $(0,0,0)$, $\frac{a}{2}(\hat{x}+\hat{y})$, $\frac{a}{2}(\hat{y}+\hat{z})$, $\frac{a}{2}(\hat{z}+\hat{x})$, $\frac{a}{4}(\hat{x}+\hat{y}+\hat{z})$, $\frac{a}{4}(-\hat{x}-\hat{y}+\hat{z})$, $\frac{a}{4}(\hat{x}-\hat{y}-\hat{z})$, $\frac{a}{4}(-\hat{x}+\hat{y}-\hat{z})$. (a)

The structure factor $S = \sum_j f_j e^{-i\vec{G}\cdot\vec{r_j}}$,

$$\vec{G} = v_1\vec{b_1} + v_2\vec{b_2} + v_3\vec{b_3} = \frac{2\pi}{a}(v_1\hat{x} + v_2\hat{y} + v_3\hat{z})$$

and $f_j = f$ (all the atoms are the same).

$$S = f(1 + e^{-i\vec{G}\cdot\frac{a}{2}(\hat{x}+\hat{y})} + e^{-i\vec{G}\cdot\frac{a}{2}(\hat{y}+\hat{z})} + e^{-i\vec{G}\cdot\frac{a}{2}(\hat{z}+\hat{x})}$$

$$+e^{-i\vec{G}\cdot\frac{a}{4}(\hat{x}+\hat{y}+\hat{z})} + e^{-i\vec{G}\cdot\frac{a}{4}(-\hat{x}-\hat{y}+\hat{z})} + e^{-i\vec{G}\cdot\frac{a}{4}(\hat{x}-\hat{y}-\hat{z})} + e^{-i\vec{G}\cdot\frac{a}{4}(-\hat{x}+\hat{y}-\hat{z})})$$

$$= f(1 + e^{-i\pi(v_1+v_2)} + e^{-i\pi(v_2+v_3)} + e^{-i\pi(v_3+v_1)} + e^{-i\frac{\pi}{2}(v_1+v_2+v_3)}$$

$$+e^{-i\frac{\pi}{2}(-v_1-v_2+v_3)} + e^{-i\frac{\pi}{2}(v_1-v_2-v_3)} + e^{-i\frac{\pi}{2}(-v_1+v_2-v_3)})$$

$$= f[(1 + e^{-i\pi(v_1+v_2)} + e^{-i\pi(v_2+v_3)} + e^{-i\pi(v_3+v_1)})$$

$$+e^{i\frac{\pi}{2}(v_1+v_2+v_3)}(1 + e^{i\pi(v_1+v_2)} + e^{-i\pi(v_2+v_3)} + e^{i\pi(v_3+v_1)}]$$

Since $e^{-i\pi v} = e^{-i\pi v}e^{i2\pi v} = e^{i\pi v}$ for $v = integer$,

$$S = f(1 + e^{-i\pi(v_1+v_2)} + e^{-i\pi(v_2+v_3)} + e^{-i\pi(v_3+v_1)})(1 + e^{i\frac{\pi}{2}(v_1+v_2+v_3)})$$

(b)

So the zeros are

(i)

$$1 + e^{-i\pi(v_1+v_2)} + e^{-i\pi(v_2+v_3)} + e^{-i\pi(v_3+v_1)} = 0$$

This means two of $e^{-i\pi(v_i+v_j)}$ are -1 and one is +1, i.e. two of $v_i + v_j$ are odd and one is even. It is possible only when two of v_1, v_2, v_3 are even and the remaining one is odd or two of v_1, v_2, v_3 are odd and the remaining one is even.

(ii)

$$1 + e^{i\frac{\pi}{2}(v_1+v_2+v_3)} = 0$$

$$\Rightarrow \frac{1}{2}(v_1 + v_2 + v_3) = odd \Rightarrow v_1 + v_2 + v_3 = 2 \times (odd)$$

The allowed reflections are anything but (i) and (ii).

(1) All of v_1, v_2, v_3 are odd.

(2) All of v_1, v_2, v_3 are even. But if $v_1 + v_2 + v_3 = 2 \times (odd)$, S still vanishes.

Thus $v_1 + v_2 + v_3$ needs to be $2 \times (even)$. i.e. $v_1 + v_2 + v_3 = 4n$ when all of v_1, v_2, v_3 are even.

Diamond described as fcc with 2 atoms/cell:

The diamond structure can be described as a face centered cubic lattice with the basis $(0,0,0), \frac{a}{4}(\hat{x}+\hat{y}+\hat{z})$.

The reciprocal lattice is bcc with primitive vectors $\vec{b_1} = \frac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z})$, $\vec{b_2} = \frac{2\pi}{a}(+\hat{x}-\hat{y}+\hat{z})$, $\vec{b_3} = \frac{2\pi}{a}(+\hat{x}+\hat{y}-\hat{z})$. The reciprocal lattice vectors are:

$$\vec{G} = m_1\vec{b_1}+m_2\vec{b_2}+m_3\vec{b_3} = \frac{2\pi}{a}[(-m_1+m_2+m_3)\hat{x}+(m_1-m_2+m_3)\hat{y}+(m_1+m_2-m_3)\hat{z})$$

This can be written as

$$\vec{G} = \frac{2\pi}{a}[(v_1\hat{x}+v_2\hat{y}+v_3\hat{z}),$$

where the integers (v_1, v_2, v_3) are all odd or all even. The restriction to all odd or all even integers can be seen by considering a bcc lattice as a simple cubic lattice (the even integers) with body centers (the odd integers).

The structure factor $S = \sum_j f_j e^{-i\vec{G}\cdot\vec{r_j}}$ with $f_j = f$ since the two atoms are the same. Thus

$$S = f(1 + e^{-i\vec{G}\cdot\frac{a}{4}(\hat{x}+\hat{y}+\hat{z})}$$

This is zero if $e^{-i\vec{G}\cdot\frac{a}{4}(\hat{x}+\hat{y}+\hat{z})} = -1$, which means $\vec{G}\cdot\frac{a}{4}(\hat{x}+\hat{y}+\hat{z}) = (2n+1)\pi$, i.e., an odd integer times π. Thus

$$\frac{\pi}{2}[v_1 + v_2 + v_3] = (2n+1)\pi$$

or

$$v_1 + v_2 + v_3 = 4n + 2$$

where n is an integer. Since the v's are all odd or all even, the only cases where $S = 0$ are they are even and do not sum to a multiple of 4. For example, the (200) and 222 peaks are missing in Figure 18, whereas they would be present in a fcc crystal with one atom/cell.

The vectors with do not satisfy this condition are "allowed" reflections. Clearly this includes all cases where the v's are all odd and the case where $v_1 + v_2 + v_3 = 4n$.