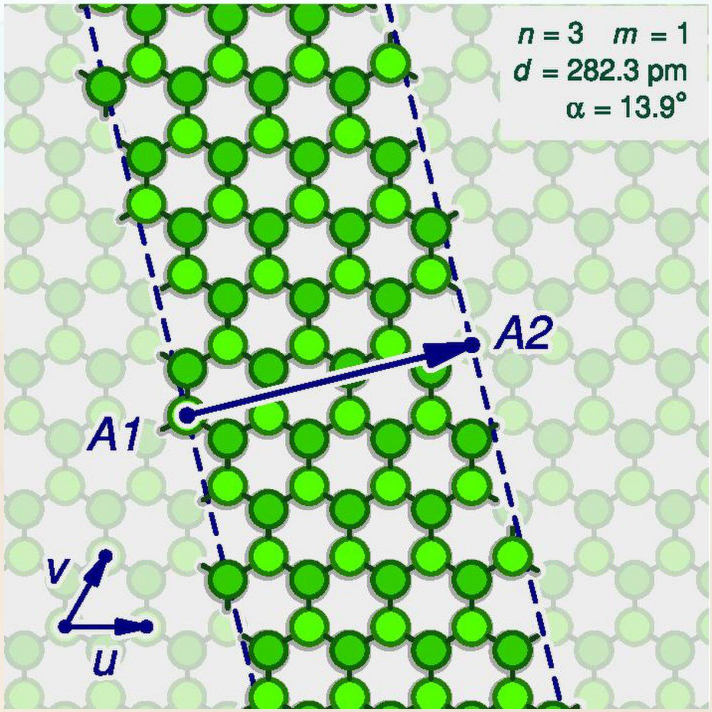
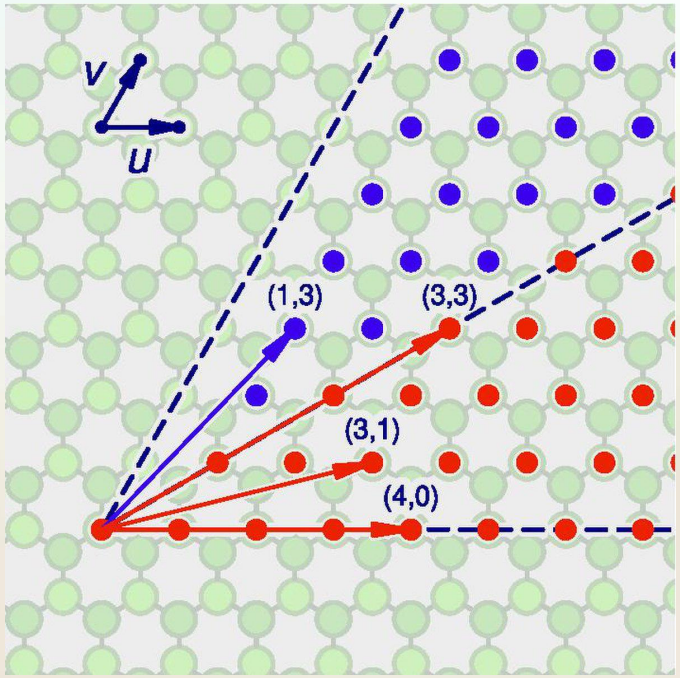
Lecture IV
Problems & Discussion

Yu-Jun Zhao
Department of Physics, SCUT

www.compphys.cn/~zhaoyj/lectures/

3. How to describe a structure of carbon nanotube?





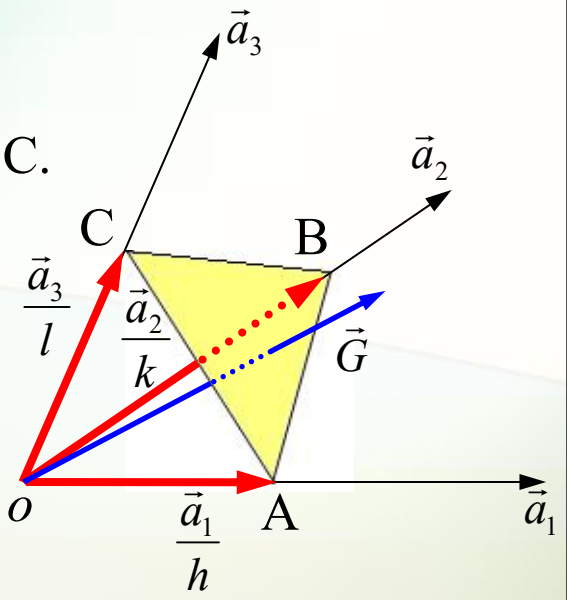
Chp 2.

1. *Interplanar separation.* Consider a plane hkl in a crystal lattice. (a) Prove that the reciprocal lattice vector $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$ is perpendicular to this plane. (b) Prove that the distance between two adjacent parallel planes of the lattice is $d(hkl) = 2\pi/|\mathbf{G}|$. (c) Show for a simple cubic lattice that $d^2 = a^2/(h^2 + k^2 + l^2)$.

Prove:

The plane (*hkl*) intercepts the axes at point A, B, and C.

$$\overrightarrow{oA} = \frac{\vec{a}_1}{h} \; ; \; \overrightarrow{oB} = \frac{\vec{a}_2}{k} \; ; \; \overrightarrow{oC} = \frac{\vec{a}_3}{l} \; .$$



then $\overrightarrow{AB} = \overrightarrow{oB} - \overrightarrow{oA} = \frac{\vec{a}_2}{k} - \frac{\vec{a}_1}{h}$.

$$\overrightarrow{AB} \cdot \vec{G} = \left(\frac{\vec{a}_2}{k} - \frac{\vec{a}_1}{h} \right) \cdot (h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3)$$

$$= \frac{h}{k}\vec{a}_2 \cdot \vec{b}_1 + \vec{a}_2 \cdot \vec{b}_2 + \frac{l}{k}\vec{a}_3 \cdot \vec{b}_2 - \vec{a}_1 \cdot \vec{b}_1 - \frac{k}{h}\vec{a}_1 \cdot \vec{b}_2 - \frac{l}{h}\vec{a}_1 \cdot \vec{b}_3$$

$$= 0$$

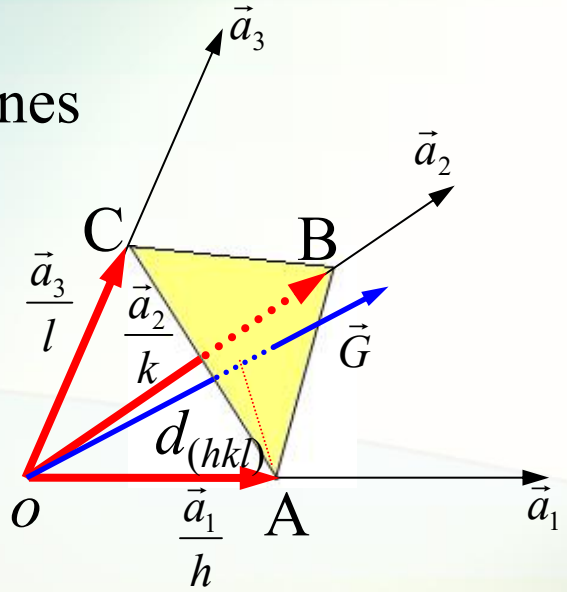
$$\overrightarrow{AB} \perp \vec{G}$$

In the same way, we can obtain $\overrightarrow{AC} \perp \vec{G}$ and $\overrightarrow{BC} \perp \vec{G}$.

So $\vec{G}$ is perpendicular to (*hkl*) plane.

The distance between two adjacent (*hkl*) planes

$$d_{(hkl)} = \overrightarrow{oA} \cdot \hat{G} = \frac{\vec{a}_1}{h} \cdot \frac{\vec{G}}{|G|} = \frac{2\pi}{|G|}$$



For a simple cubic lattice

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

$$|G| = \frac{2\pi}{a}\left(h^2 + k^2 + l^2\right)^{1/2}$$

Then $$d_{(hkl)} = \frac{a}{\left(h^2 + k^2 + l^2\right)^{1/2}}$$

Chp 2.

2. ***Hexagonal space lattice.*** The primitive translation vectors of the hexagonal space lattice may be taken as

$$\mathbf{a}_1 = (3^{1/2}a/2)\hat{\mathbf{x}} + (a/2)\hat{\mathbf{y}} \quad ; \qquad \mathbf{a}_2 = -(3^{1/2}a/2)\hat{\mathbf{x}} + (a/2)\hat{\mathbf{y}} \quad ; \qquad \mathbf{a}_3 = c\hat{\mathbf{z}} \quad .$$

(a) Show that the volume of the primitive cell is $(3^{1/2}/2)a^2c$.

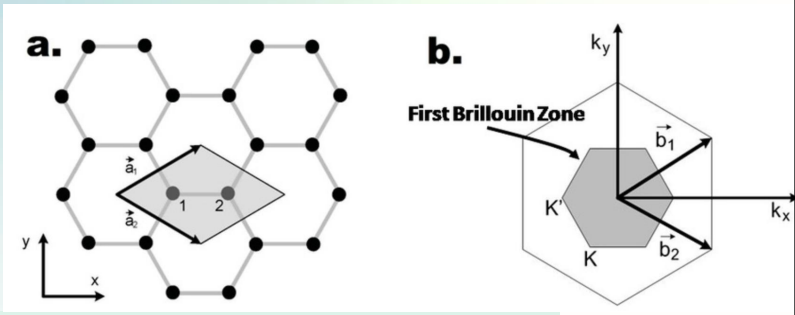
(b) Show that the primitive translations of the reciprocal lattice are

$$\mathbf{b}_1 = (2\pi/3^{1/2}a)\hat{\mathbf{x}} + (2\pi/a)\hat{\mathbf{y}} \quad ; \qquad \mathbf{b}_2 = -(2\pi/3^{1/2}a)\hat{\mathbf{x}} + (2\pi/a)\hat{\mathbf{y}} \quad ; \qquad \mathbf{b}_3 = (2\pi/c)\hat{\mathbf{z}} \quad ,$$

so that the lattice is its own reciprocal, but with a rotation of axes.

(c) Describe and sketch the first Brillouin zone of the hexagonal space lattice.

1. Hexagonal space lattice



a) the volume of the primitive cell is

$$
\begin{aligned}
V_C &= \vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3 \\
&= [(3^{1/2} a/2)\hat{x} + (a/2)\hat{y}] \cdot [-(3^{1/2} a/2)\hat{x} + (a/2)\hat{y}] \times c\hat{z} \\
&= c(3^{1/2} a/2)(a/2)(\hat{x} \cdot \hat{y} \times \hat{z}) - c(3^{1/2} a/2)(a/2)(\hat{y} \cdot \hat{x} \times \hat{z}) \\
&= \frac{3^{1/2}}{2} a^2 c
\end{aligned}
$$

b) the reciprocal lattice

$$
\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{V_c} = 2\pi \left(\frac{3^{1/2}}{2} a^2 c \right)^{-1} \left(-\frac{3^{1/2} a}{2} \hat{x} + \frac{a}{2} \hat{y} \right) \times c\hat{z}
$$

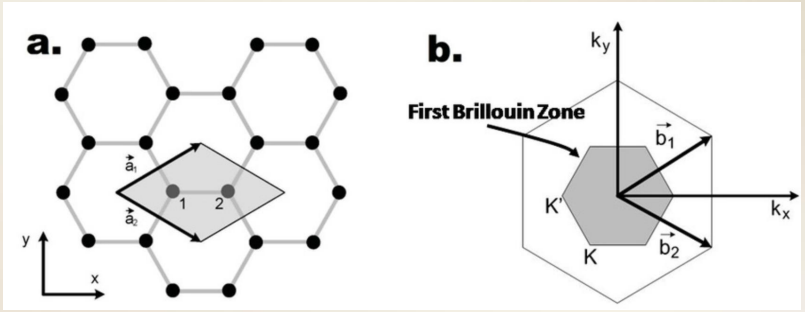
$$
= \frac{2\pi}{3^{1/2} a} \hat{x} + \frac{2\pi}{a} \hat{y}
$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{V_c} = 2\pi \left(\frac{3^{1/2}}{2} a^2 c \right)^{-1} c\hat{z} \times \left(\frac{3^{1/2} a}{2} \hat{x} + \frac{a}{2} \hat{y} \right)$$

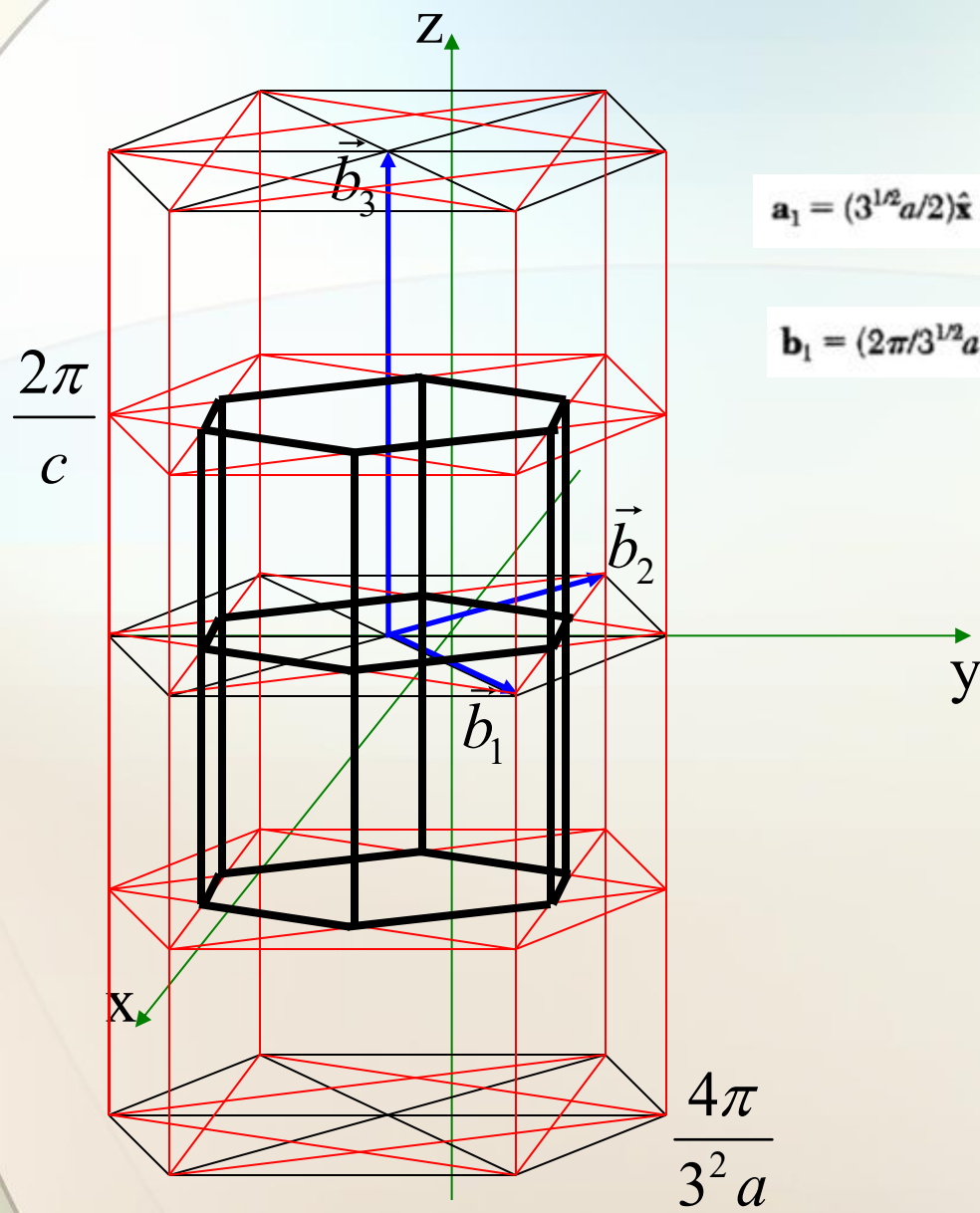
$$= -\frac{2\pi}{3^{1/2} a} \hat{x} + \frac{2\pi}{a} \hat{y}$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{V_c} = 2\pi \left(\frac{3^{1/2}}{2} a^2 c \right)^{-1} \left(\frac{3^{1/2} a}{2} \hat{x} + \frac{a}{2} \hat{y} \right) \times \left(-\frac{3^{1/2} a}{2} \hat{x} + \frac{a}{2} \hat{y} \right)$$

$$= 2\pi \left(\frac{3^{1/2}}{2} a^2 c \right)^{-1} \frac{3^{1/2} a^2}{2} \hat{z} = \frac{2\pi}{c} \hat{z}$$

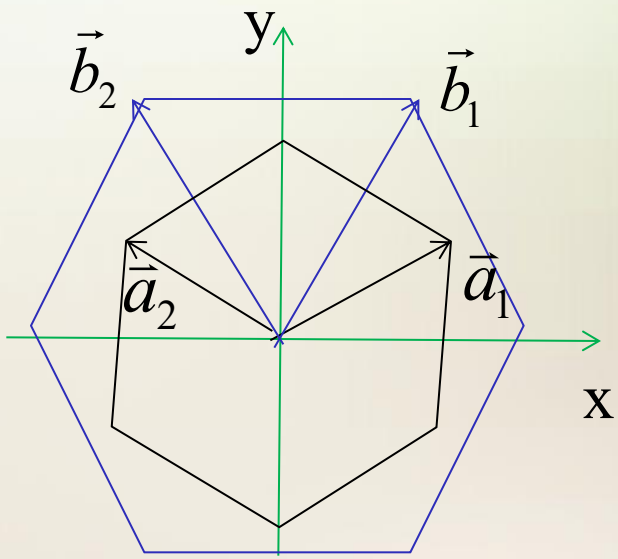


c) the first Brillouin zone



$\mathbf{a}_1 = (3^{1/2}a/2)\hat{\mathbf{x}} + (a/2)\hat{\mathbf{y}}$; $\mathbf{a}_2 = -(3^{1/2}a/2)\hat{\mathbf{x}} + (a/2)\hat{\mathbf{y}}$

$\mathbf{b}_1 = (2\pi/3^{1/2}a)\hat{\mathbf{x}} + (2\pi/a)\hat{\mathbf{y}}$; $\mathbf{b}_2 = -(2\pi/3^{1/2}a)\hat{\mathbf{x}} + (2\pi/a)\hat{\mathbf{y}}$



Chp 2.

4. *Width of diffraction maximum.* We suppose that in a linear crystal there are identical point scattering centers at every lattice point $\boldsymbol{\rho}_m = m\mathbf{a}$, where m is an integer. By analogy with (20), the total scattered radiation amplitude will be proportional to $F = \Sigma \exp[-im\mathbf{a} \cdot \Delta\mathbf{k}]$. The sum over M lattice points is

$$F = \frac{1 - \exp[-iM(\mathbf{a} \cdot \Delta\mathbf{k}]}{1 - \exp[-i(\mathbf{a} \cdot \Delta\mathbf{k})]} ,$$

by the use of the series

$$\sum_{m=0}^{M-1} x^m = \frac{1 - x^M}{1 - x} .$$

(a) The scattered intensity is proportional to $|F|^2$. Show that

$$|F|^2 \equiv F^*F = \frac{\sin^2 \frac{1}{2} M(\mathbf{a} \cdot \Delta\mathbf{k})}{\sin^2 \frac{1}{2} (\mathbf{a} \cdot \Delta\mathbf{k})} .$$

(b) We know that a diffraction maximum appears when $\mathbf{a} \cdot \Delta\mathbf{k} = 2\pi h$, where h is an integer. We change $\Delta\mathbf{k}$ slightly and define ϵ in $\mathbf{a} \cdot \Delta\mathbf{k} = 2\pi h + \epsilon$ such that ϵ gives the position of the first zero in $\sin \frac{1}{2} M(\mathbf{a} \cdot \Delta\mathbf{k})$. Show that $\epsilon = 2\pi/M$, so that the width of the diffraction maximum is proportional to $1/M$ and can be extremely narrow for macroscopic values of M. The same result holds true for a three-dimensional crystal.

2.4 Width of diffraction maximum

a) scattered intensity

$$F = \frac{1-\exp[-iM(\vec{a}\cdot\Delta\vec{k})]}{1-\exp[-i(\vec{a}\cdot\Delta\vec{k})]}$$

$$F^* = \frac{1-\exp[iM(\vec{a}\cdot\Delta\vec{k})]}{1-\exp[i(\vec{a}\cdot\Delta\vec{k})]}$$

$$|F|^2 \equiv F^*F = \frac{1-\exp[iM(\vec{a}\cdot\Delta\vec{k})]}{1-\exp[i(\vec{a}\cdot\Delta\vec{k})]}\frac{1-\exp[-iM(\vec{a}\cdot\Delta\vec{k})]}{1-\exp[-i(\vec{a}\cdot\Delta\vec{k})]}$$

$$= \frac{2-\exp[-iM(\vec{a}\cdot\Delta\vec{k})]-\exp[iM(\vec{a}\cdot\Delta\vec{k})]}{2-\exp[-i(\vec{a}\cdot\Delta\vec{k})]-\exp[i(\vec{a}\cdot\Delta\vec{k})]}$$

$$= \frac{2-2\cos[M(\vec{a}\cdot\Delta\vec{k})]}{2-2\cos(\vec{a}\cdot\Delta\vec{k})} = \frac{\sin^2[M(\vec{a}\cdot\Delta\vec{k})/2]}{\sin^2[(\vec{a}\cdot\Delta\vec{k})/2]}$$

b) width of diffraction maximum

a slight change of Δk results a small change ε in $\vec{a}\cdot\Delta\vec{k}$

$$\vec{a}\cdot\Delta\vec{k} = 2\pi h + \varepsilon$$

$$\sin^2[M(\vec{a}\cdot\Delta\vec{k})/2]$$

$$= \sin^2[M(2\pi h + \varepsilon)/2]$$

$$= \sin^2(Mh\pi + M\varepsilon/2)$$

$$= \sin^2(M\varepsilon/2)$$

the first zero gives $M\varepsilon/2 = \pi$

i.e. $\varepsilon = 2\pi/M$

The width of the diffraction maximum is inverse to M, where M is the number lattice points. For nanostructures the width of the diffraction maximum is quite big. From XDR, one can estimate the size of the nanostructures.

Chp 2.

5. ***Structure factor of diamond.*** The crystal structure of diamond is described in Chapter 1. The basis consists of eight atoms if the cell is taken as the conventional cube. (a) Find the structure factor S of this basis. (b) Find the zeros of S and show that the allowed reflections of the diamond structure satisfy $v_1 + v_2 + v_3 = 4n$, where all indices are even and n is any integer, or else all indices are odd (Fig. 18). (Notice that h, k, l may be written for v_1, v_2, v_3 and this is often done.)

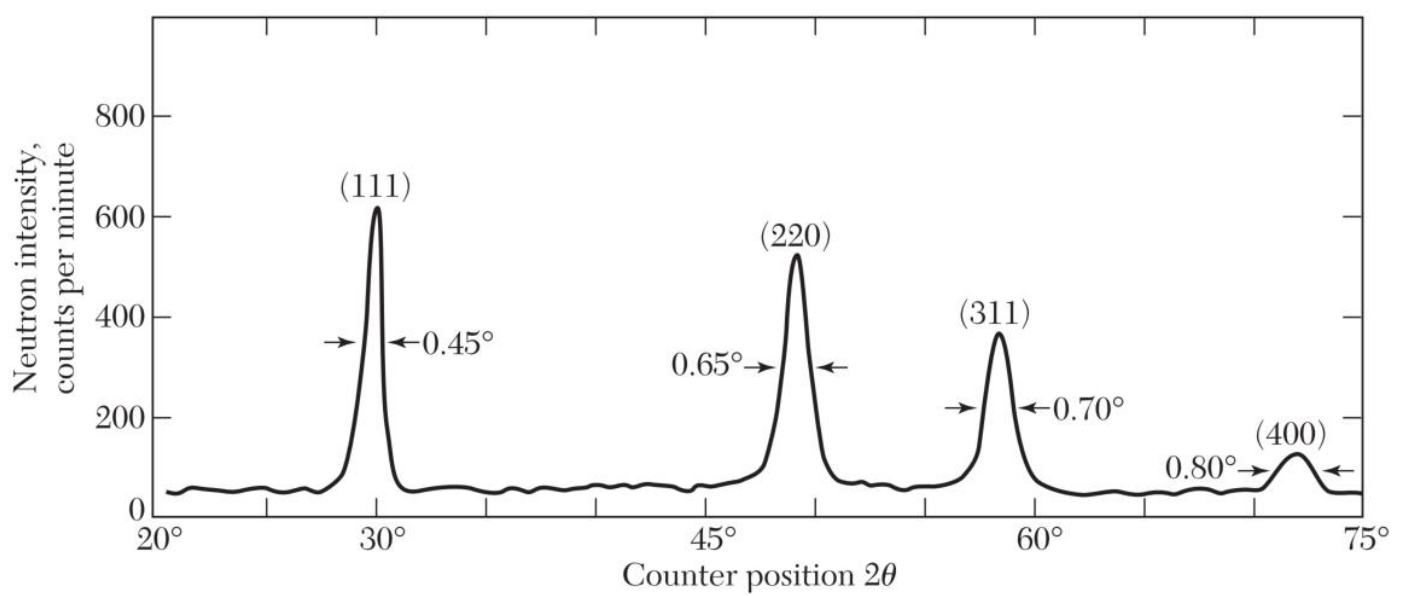


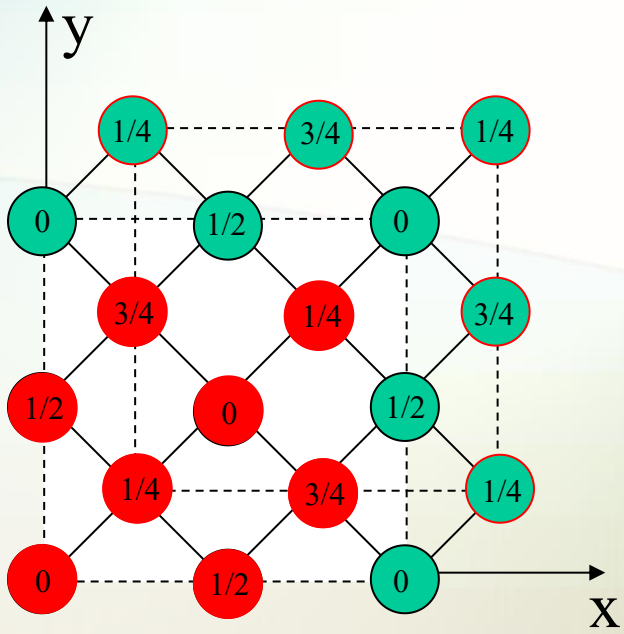
Figure 18 Neutron diffraction pattern for powdered diamond. (After G. Bacon.)

2.5 Structure factor of diamond

There are eight carbon atoms in the conventional cell,

(0 0 0), (¼ ¼ ¼), (½ 0 ½),(0 ½ ½),

(½ ½ 0),(¾ ¼ ¾), (¼ ¾ ¾), (¾ ¾ ¼),



structure factor

$$S = \sum_j f_j \exp(-i\vec{r}_j \cdot \vec{G})$$

$$= f \sum_j \exp[-2\pi i(x_j h + y_j k + z_j l)]$$

$$= f\{1 + \exp[-i\pi/2(h+k+l)] + \exp[-i\pi(h+k)]$$
$$+ \exp[-i\pi(k+l)] + \exp[-i\pi(h+l)] + \exp[-i\pi/2(3h+k+3l)]$$
$$+ \exp[-i\pi/2(h+3k+3l)] + \exp[-i\pi/2(h+3k+3l)]\}$$

$$= f\{1 + \exp[-i\pi/2(h+k+l)]\}\{1 + \exp[-i\pi(h+k)]$$
$$+ \exp[-i\pi(h+l)] + \exp[-i\pi(k+l)]\}$$

$$S = f\{1+\exp[-i\pi/2(h+k+l)]\}\{1+\exp[-i\pi(h+k)] + \exp[-i\pi(h+l)] + \exp[-i\pi(k+l)]\}$$

S = 0 when:

1) Not all *h*, *k*, *l* are evens (or odds)

2) $\exp[-i\pi/2(h+k+l)] = -1$

i.e. $h + k + l = 4n + 2$

S ≠ 0 when:

1) All *h*, *k*, *l* are odd integers

$$S = 4f(1 \pm i)$$

2) All *h*, *k*, *l* are even integers and $h + k + l = 4n$

$$S = 8f$$

Chap 2. Discussion of powder diffraction

PROBLEMS

1. Powder specimens of three different monatomic cubic crystals are analyzed with a Debye-Scherrer camera. It is known that one sample is face-centered cubic, one is body-centered cubic, and one has the diamond structure. The approximate positions of the first four diffraction rings in each case are (see Figure 6.13):

VALUES OF ϕ FOR SAMPLES

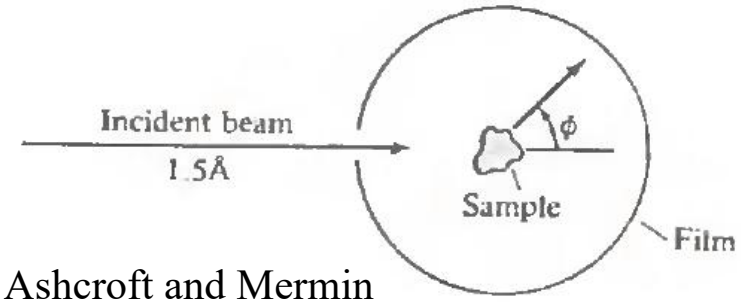
A	*B*	*C*
42.2°	28.8°	42.8°
49.2	41.0	73.2
72.0	50.8	89.0
87.3	59.6	115.0

(a) Identify the crystal structures of *A*, *B*, and *C*.

(b) If the wavelength of the incident X-ray beam is 1.5 Å, what is the length of the side of the conventional cubic cell in each case?

(c) If the diamond structure were replaced by a zincblende structure with a cubic unit cell of the same side, at what angles would the first four rings now occur?

Figure 6.13
Schematic view of a Debye-Scherrer camera. Diffraction peaks are recorded on the film strip.

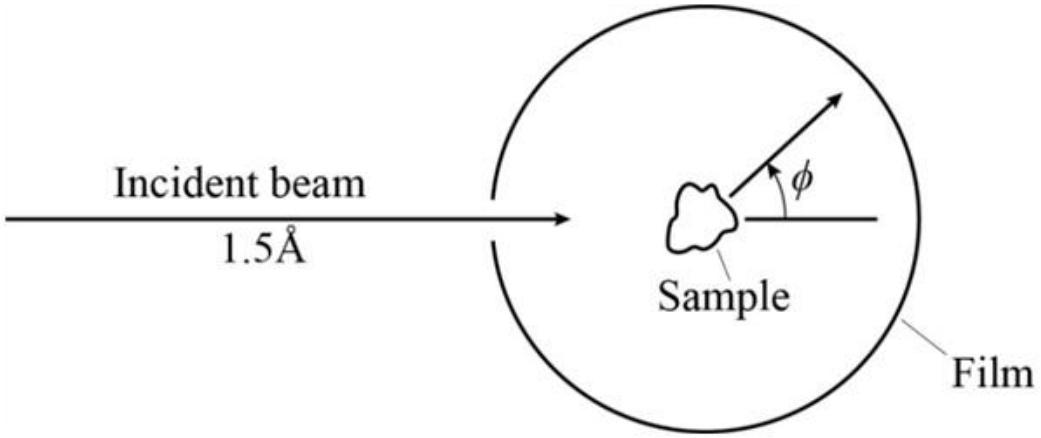


Solid State Physics, Ashcroft and Mermin

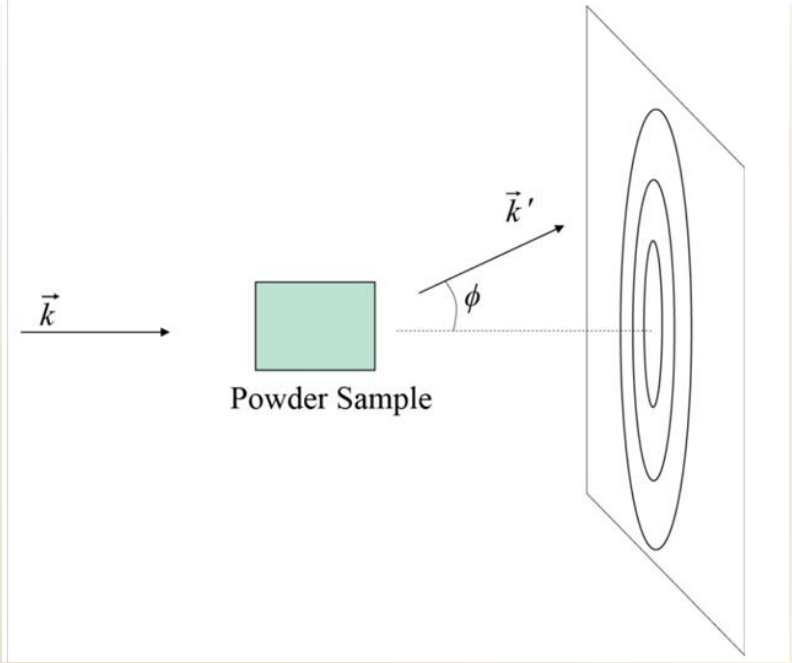
(a)

Powder samples of three different monatomic cubic crystals are examined with a Debye-Scherrer camera.

Schematic view of a Debye-Scherrer camera showing recorded diffraction peaks on the film strip is shown below in figure 1:



Diffraction rings are expected for Debye-Scherrer X-ray diffraction from a powder sample as shown below in figure



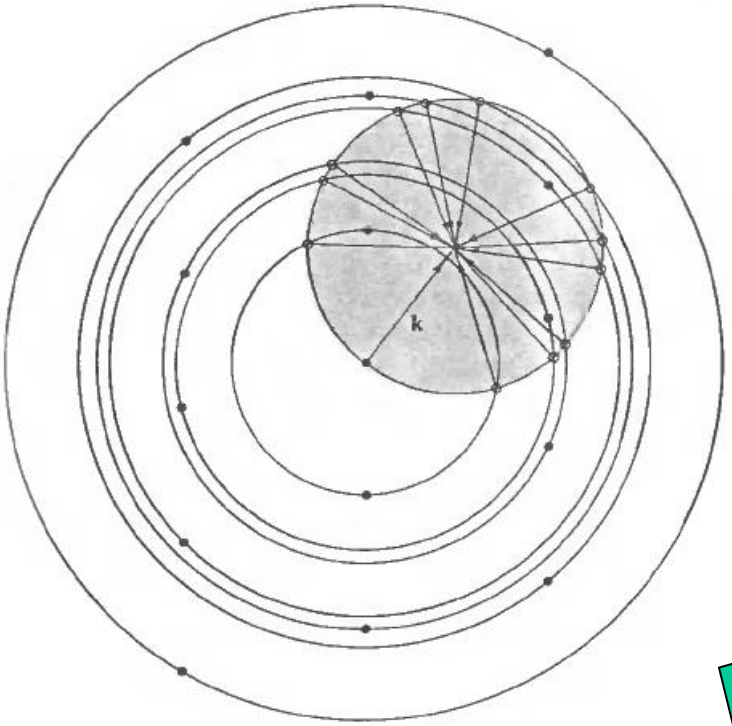
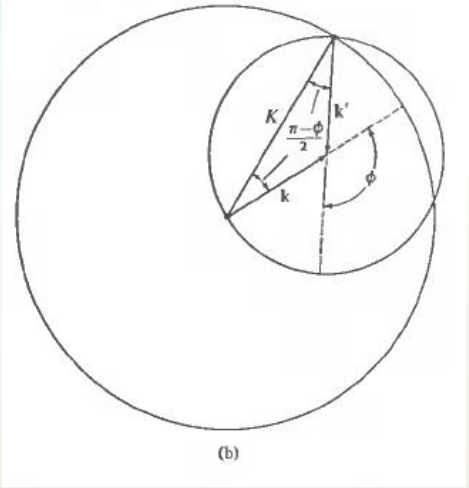
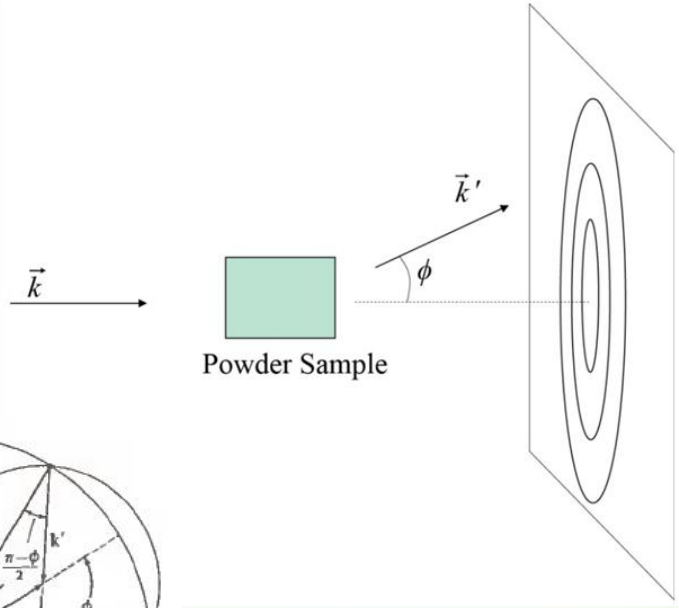


Figure 6.9
The Ewald construction for the rotating-crystal method. For simplicity a case is shown in which the incident wave vector lies in a lattice plane, and the axis of rotation is perpendicular to that plane. The concentric circles are the orbits swept out under the rotation by the reciprocal lattice vectors lying in the plane perpendicular to the axis containing k. Each intersection of such a circle with the Ewald sphere gives the wave vector of a Bragg reflected ray. (Additional Bragg reflected wave vectors associated with reciprocal lattice vectors in other planes are not shown.)



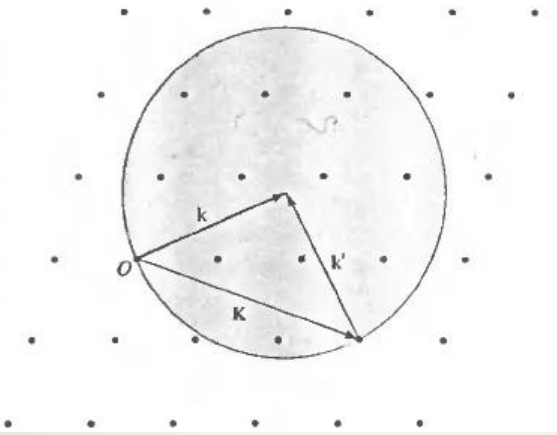


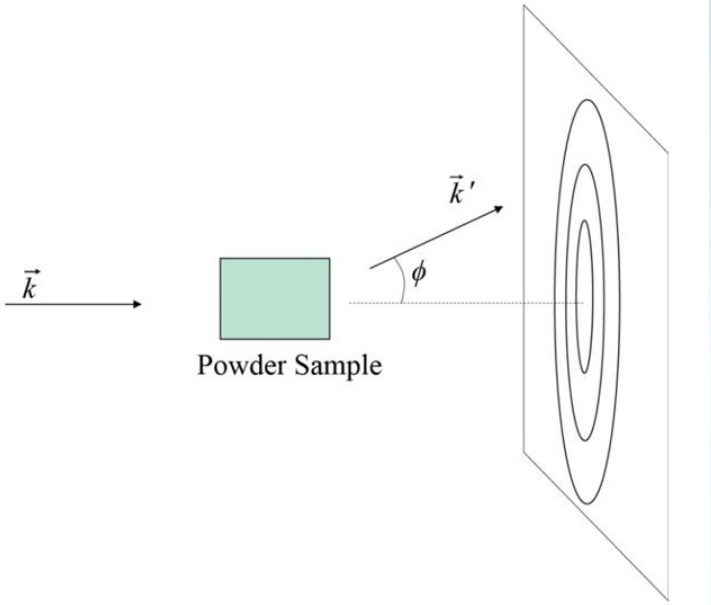
Laue condition

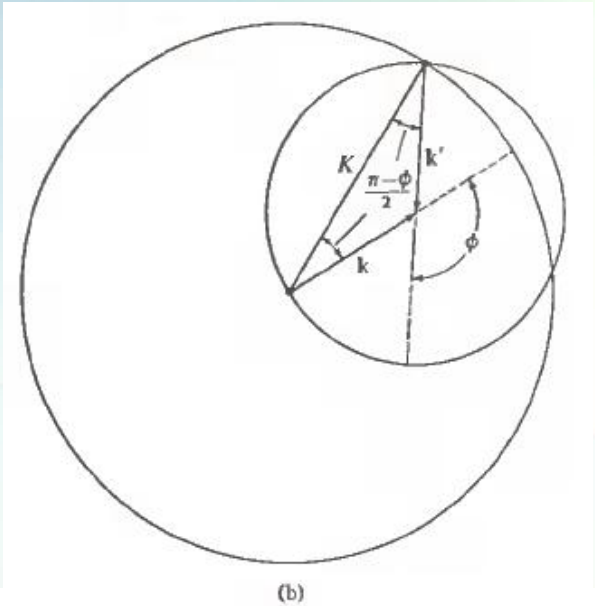
$$k = |\mathbf{k} - \mathbf{K}|.$$

$$\mathbf{k} \cdot \hat{\mathbf{K}} = \tfrac{1}{2}K;$$

Figure 6.7
The Ewald construction. Given the incident wave vector **k**, a sphere of radius k is drawn about the point **k**. Diffraction peaks corresponding to reciprocal lattice vectors **K** will be observed only if **K** gives a reciprocal lattice point on the surface of the sphere. Such a reciprocal lattice vector is indicated in the figure, together with the wave vector **k′** of the Bragg reflected ray.







(b)

Step 2 of 9

From the Laue condition that is $\vec{k} - \vec{k}' = \vec{K}$, $\vec{K}$ stands for reciprocal lattice vector, it is known that for a crystal structure corresponding to a particular Bravais lattice, the diffraction rings should be seen when the scattering angle ϕ satisfies the below expression:

$$K = 2k \sin\frac{\phi}{2}$$

In the above expression K stands for magnitude of a vector in the reciprocal lattice and k represents magnitude of a wave vector of the diffracted X-rays.

Also, to check probable line extinction it is desired to compute structure factor when dealing with a lattice having a basis like diamond.

Step 3 of 9

The given values of ϕ for the samples A, B and C are shown in the below table.

A	*B*	*C*
42.2°	28.8°	42.8°
49.2	41.0	73.2
70.0	50.8	89.0
87.3	59.6	115.0

Table 1

Firstly determine the magnitudes of the shortest vectors in the reciprocal lattice of the body centered cubic structures and face centered cubic structures.

Step 4 of 9

So, for a crystal with face centered cubic structures, the reciprocal lattice is body centered cubic structures, and the shortest reciprocal lattice vectors and their magnitudes are as follows:

$$\vec{K}_1 = b\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$$

$$K_1 = b\sqrt{\left(\frac{1}{2}\right)^2+\left(\frac{1}{2}\right)^2+\left(\frac{1}{2}\right)^2}$$

$$= b\sqrt{\frac{1}{4}+\frac{1}{4}+\frac{1}{4}}$$

$$= b\frac{\sqrt{3}}{2}$$

$$\vec{K}_2 = b(1,0,0)$$

$$K_2 = b\sqrt{(1)^2+(0)^2+(0)^2}$$

$$= b\sqrt{1+0+0}$$

$$= b$$

$$\vec{K}_3 = b(1,1,0)$$

$$K_3 = b\sqrt{(1)^2+(1)^2+(0)^2}$$

$$= b\sqrt{1+1+0}$$

$$= b\sqrt{2}$$

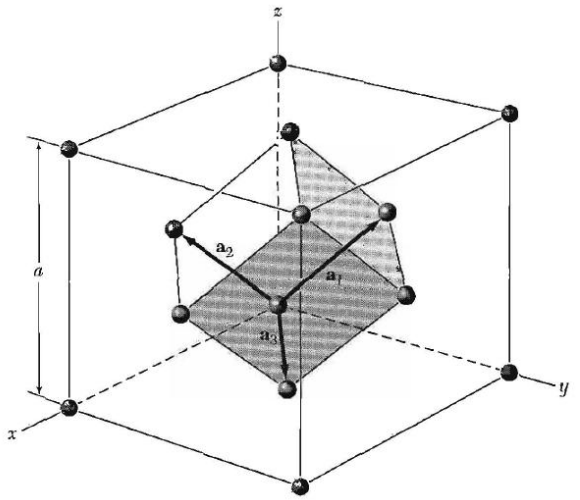
$$\vec{K}_4 = b\left(\frac{1}{2},\frac{1}{2},\frac{3}{2}\right)$$

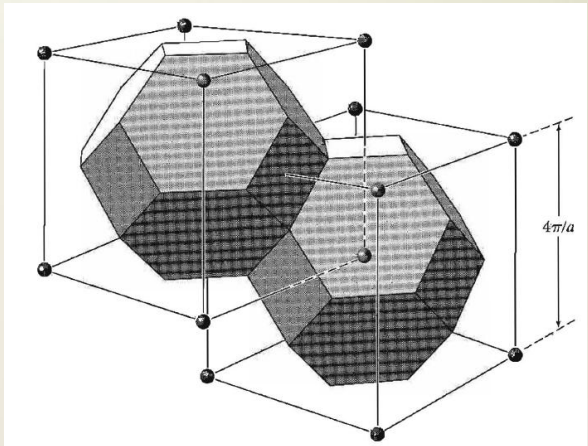
$$K_4 = b\sqrt{\left(\frac{1}{2}\right)^2+\left(\frac{1}{2}\right)^2+\left(\frac{3}{2}\right)^2}$$

$$= b\sqrt{\frac{1}{4}+\frac{1}{4}+\frac{9}{4}}$$

$$= b\frac{\sqrt{11}}{2}$$

Here, the value of b is $\frac{4\pi}{a}$.





Step 5 of 9

A crystal with diamond structure is described by the face centered cubic structure Bravais lattice by the following below vectors;

$$\vec{v}_1 = 0$$

$$\vec{v}_2 = a\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right)$$

As diamond is monatomic, the structure factor $(S_{\vec{K}})$ is given by the following below expression:

$$S_{\vec{K}} = 1 + e^{i\vec{K}\cdot\vec{v}_2}$$

Hence, for odd multiple of $\vec{K}\cdot\vec{v}_2$ the peaks will not occur.

So calculate $\vec{K}\cdot\vec{v}_2$ for the reciprocal lattice vectors $\vec{K}_1$ $\vec{K}_2$, $\vec{K}_3$ and $\vec{K}_4$

$$\vec{v}_2\cdot\vec{K}_1 = \frac{3\pi}{2}$$

$$\vec{v}_2\cdot\vec{K}_2 = \pi$$

$$\vec{v}_2\cdot\vec{K}_3 = 2\pi$$

$$\vec{v}_2\cdot\vec{K}_4 = \frac{5\pi}{2}$$

The 4 shortest reciprocal lattice vectors:

$$\vec{K}_1 = b\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$$

$$\vec{K}_2 = b(1,0,0)$$

$$\vec{K}_3 = b(1,1,0)$$

$$\vec{K}_4 = b\left(\frac{1}{2}, \frac{1}{2}, \frac{3}{2}\right)$$

Hence, K_1, K_3 and K_4 will generate a diffraction ring for diamond but K_2 will not therefore determine more reciprocal lattice for diamond with greater length than K_4.

$$\vec{K}_5 = b(1,1,1)$$

$$K_5 = b\sqrt{1^2+1^2+1^2}$$

$$= b\sqrt{1+1+1}$$

$$= b\sqrt{3}$$

$$\vec{K}_6 = b(2,0,0)$$

$$K_6 = b\sqrt{2^2+0^2+0^2}$$

$$= b\sqrt{4+0+0}$$

$$= b2$$

Here, K_5 will not generate a diffraction ring as $\vec{v}_2 \cdot \vec{K}_5 = 3\pi$ whereas K_6 will create a diffraction ring as $\vec{v}_2 \cdot \vec{K}_6 = 2\pi$

$$S_{\vec{K}} = 1 + e^{i\vec{K}\cdot\vec{v}_2}$$

Step 6 of 9

Lastly, for a body centered cubic crystal, the reciprocal lattice is face centered cubic structures, and the shortest reciprocal lattice vectors and their magnitudes are as follows:

$$\vec{K}_1 = b\left(\frac{1}{2},\frac{1}{2},0\right)$$

$$K_1 = b\sqrt{\left(\frac{1}{2}\right)^2+\left(\frac{1}{2}\right)^2+(0)^2}$$

$$= b\sqrt{\frac{1}{4}+\frac{1}{4}+0}$$

$$= b\frac{\sqrt{2}}{2}$$

$$\vec{K}_2 = b(1,0,0)$$

$$K_2 = b\sqrt{(1)^2+(0)^2+(0)^2}$$

$$= b\sqrt{1+0+0}$$

$$= b$$

$$\vec{K}_3 = b\left(1,\frac{1}{2},\frac{1}{2}\right)$$

$$K_3 = b\sqrt{(1)^2+\left(\frac{1}{2}\right)^2+\left(\frac{1}{2}\right)^2}$$

$$= b\sqrt{1+\frac{1}{4}+\frac{1}{4}}$$

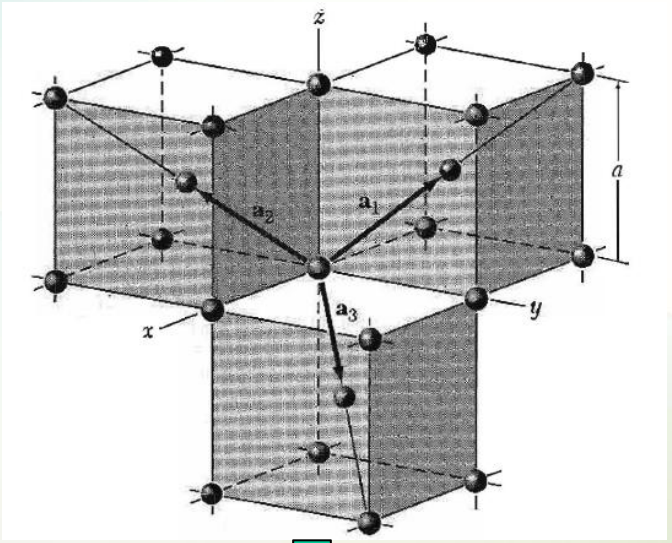
$$= b\frac{\sqrt{6}}{2}$$

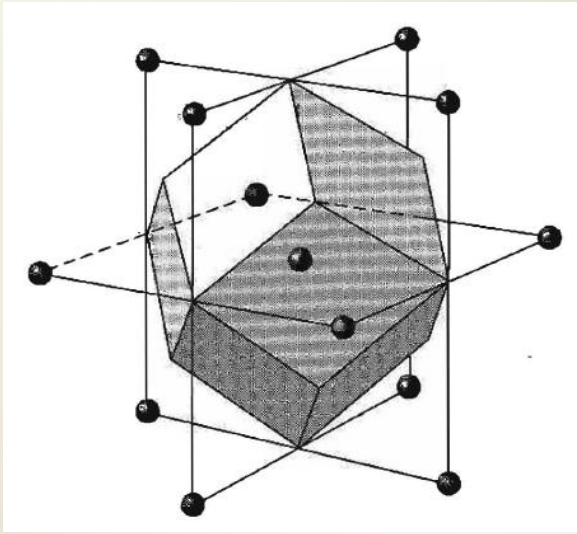
$$\vec{K}_4 = b(1,1,0)$$

$$K_4 = b\sqrt{(1)^2+(1)^2+(0)^2}$$

$$= b\sqrt{1+1+}$$

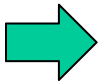
$$= b\sqrt{2}$$





The table that lists the magnitudes of the four smallest $\vec{K}$ vectors that generate diffraction for face centered cubic structures, diamond and body centered cubic structures is given below:

	FCC	Diamond	BCC
K_1	$b\frac{\sqrt{3}}{2}$	$b\frac{\sqrt{3}}{2}$	$b\frac{\sqrt{2}}{2}$
K_2	b	$b\sqrt{2}$	b
K_3	$b\sqrt{2}$	$b\frac{\sqrt{11}}{2}$	$b\frac{\sqrt{6}}{2}$
K_4	$b\frac{\sqrt{11}}{2}$	$b2$	$\sqrt{2}b$



	FCC	Diamond	BCC
$\frac{K_1}{K_1}$	1	1	1
$\frac{K_2}{K_1}$	1.15	1.63	1.41
$\frac{K_3}{K_1}$	1.63	1.91	1.73
$\frac{K_4}{K_1}$	1.91	2.31	2.00

Determine the ratio s of $\sin\frac{\phi}{2}$ for the observed ring in the tabulated form, shown below in table 4

$$K = 2k\sin\frac{\phi}{2}$$

	A	B	C
$\frac{\sin\left(\frac{\phi_1}{2}\right)}{\sin\left(\frac{\phi_1}{2}\right)}$	1	1	1
$\frac{\sin\left(\frac{\phi_2}{2}\right)}{\sin\left(\frac{\phi_1}{2}\right)}$	1.16	1.41	1.63
$\frac{\sin\left(\frac{\phi_3}{2}\right)}{\sin\left(\frac{\phi_1}{2}\right)}$	1.63	1.72	1.92
$\frac{\sin\left(\frac{\phi_4}{2}\right)}{\sin\left(\frac{\phi_1}{2}\right)}$	1.92	2.00	2.31

	FCC	Diamond	BCC
$\frac{K_1}{K_1}$	1	1	1
$\frac{K_2}{K_1}$	1.15	1.63	1.41
$\frac{K_3}{K_1}$	1.63	1.91	1.73
$\frac{K_4}{K_1}$	1.91	2.31	2.00

Step 8 of 9

(b)

Here, the wavelength of the incident X-ray beam is $1.5\ \text{Å}$. In the case of face centered cubic structure (FCC).

$$K_1 = 2k\sin\frac{\phi_1}{2}$$

Substitute corresponding values in above expression:

$$\frac{2\pi}{a}\sqrt{3} = 2\frac{2\pi}{\lambda}\sin\frac{\phi_1}{2}$$

$$a = \frac{\sqrt{3}}{2}\frac{\lambda}{\sin\frac{\phi_1}{2}}$$

$$= 3.6\ \text{Å}$$

In the case of body centered cubic structure (BCC)

$$K_1 = 2k\sin\frac{\phi_1}{2}$$

Substitute corresponding values in above expression:

$$\frac{2\pi}{a}\sqrt{2} = 2\frac{2\pi}{\lambda}\sin\frac{\phi_1}{2}$$

$$a = \frac{\sqrt{2}}{2}\frac{\lambda}{\sin\frac{\phi_1}{2}}$$

$$= 4.3\ \text{Å}$$

In the case of diamond structure

$$K_1 = 2k\sin\frac{\phi_1}{2}$$

Substitute corresponding values in above expression:

$$\frac{2\pi}{a}\sqrt{3} = 2\frac{2\pi}{\lambda}\sin\frac{\phi_1}{2}$$

$$a = \frac{\sqrt{3}}{2}\frac{\lambda}{\sin\frac{\phi_1}{2}}$$

$$= 3.6\ \text{Å}$$

Step 9 of 9

(c)

Here, the diamond structure is replaced by a zincblende structure with a cube unit cell of same side; the changed structure factor is given below;

$$S_{\vec{K}} = f_1\left(\vec{K}\right) + f_2\left(\vec{K}\right)e^{i\vec{K}\cdot v_2}$$

In the above expression f_1 and f_2 stands for atomic form factors of the two atoms in consideration.

These atoms are not identical in zincblende and $S_{\vec{K}}$ will not vanish for any $\vec{K}$.

Hence, the diffraction rings can be seen in the reciprocal lattice of FCC for all $\vec{K}'s$.

$$\frac{\sin\frac{\phi}{2}}{\sin\frac{\phi_1}{2}} = \frac{2}{\sqrt{3}}$$

$$\phi_2 = 2\sin^{-1}\frac{\sqrt{2}}{\sqrt{3}}\sin\frac{42.8}{2}$$

$$= 49.8°$$

Hence, the angle at which the first four ring will occur is $\boxed{49.8°}$.