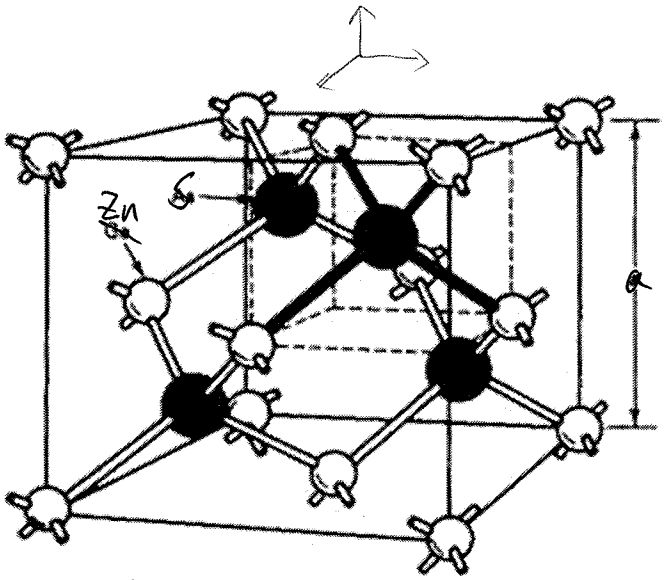
Problem Set # 6 Solutions

1. (Simon 12.3)

(a) The Bravais lattice is Face-centered cubic.

ZnS is a zincblende structure composed of two interpenetrating FCC lattice.

(b)



As shown in the figure above, the unit cell is the small box which has a 2-atom basis.

Set Zn $(0,0,0)$, then S $(\frac{1}{4},\frac{1}{4},-\frac{1}{4})$

(c) $a = 0.541$ nm

$$d(Zn-Zn) = \sqrt{(\tfrac{a}{2})^2+(\tfrac{a}{2})^2} = \frac{\sqrt{2}}{2}a = 3.83\ \text{Å}$$

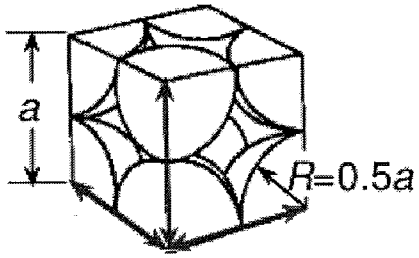
$$d(Zn-S) = \sqrt{(\tfrac{a}{4})^2+(\tfrac{a}{4})^2+(\tfrac{a}{4})^2} = \frac{\sqrt{3}}{4}a = 2.34\ \text{Å}$$

$$d(S-S) = d(Zn-Zn) = \frac{\sqrt{2}}{2}a = 3.83\ \text{Å}$$

2. (Simon 12.4)

(a) For Simple cubic lattice

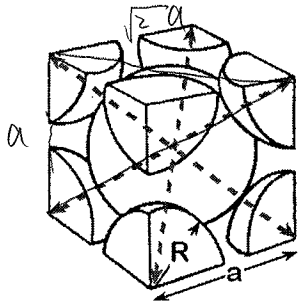
$a = 2R$



$$\frac{V_{atom}}{V_{cell}} = \frac{\frac{4}{3}\pi R^3}{(2R)^3} = \frac{\pi}{6} \approx 0.52$$

(b) For BCC lattice

The diagonal length is $\sqrt{3}a$,



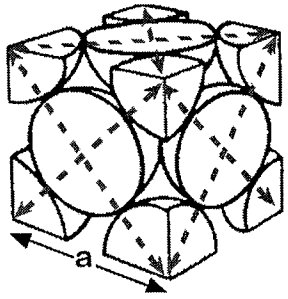
$$\sqrt{3}a = R + 2R + R$$

$$a = \frac{4}{\sqrt{3}}R$$

$$\frac{V_{atom}}{V_{cell}} = \frac{2 \times \frac{4}{3}\pi R^3}{(\frac{4}{\sqrt{3}}R)^3} = \frac{\sqrt{3}}{8}\pi \approx 0.68$$

(c) For FCC lattice

The diagonal length on the side is $\sqrt{2}a$.



$$\sqrt{2}a = R + 2R + R$$

$$a = 2\sqrt{2}R$$

$$\frac{V_{atom}}{V_{cell}} = \frac{2 \times \frac{4}{3}\pi R^3}{(2\sqrt{2}R)^3} = \frac{\sqrt{2}}{6}\pi \approx 0.74$$

3. (Simon 12.5)

(a) In this conventional unit cell, the number of atoms is

$$8 \times \frac{1}{8} + 12 \times \frac{1}{2} + 1 = 8$$

(b) This crystal is a simple cubic lattice with 8-atom basis.

$(0, 0, 0)$

$(\frac{1}{4}, \frac{1}{2}, 0)$

$(\frac{3}{4}, \frac{1}{2}, 0)$

$(\frac{1}{2}, 0, \frac{1}{4})$

$(\frac{1}{2}, 0, \frac{3}{4})$

$(0, \frac{1}{4}, \frac{1}{2})$

$(0, \frac{3}{4}, \frac{1}{2})$

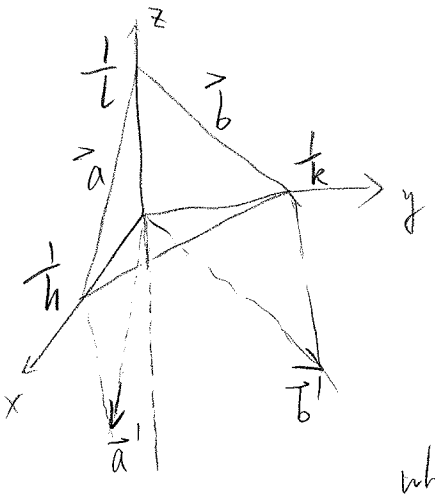
$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

4. (Simon 13.3)

(a) Crystal planes are sets of parallele planes in the lattice of each contains at least 3 non-collinear lattice points.

Miller indices are integers that define crystal plane.

(b) To confirm $[h\,k\,l] \perp (h\,k\,l)$, we just need to prove that $[h.k.l]$ perpendicular to any two lines in $(h\,k\,l)$ plane.



the direction $[h\,k\,l]$ can be written as

$$\vec{n} = h\hat{x} + k\hat{y} + l\hat{z}$$

From the figure, we chosse two lines a and b, where $\vec{a}'$ and $\vec{b}'$ are paralleld to each of them.

$$\vec{a}' = \frac{1}{h}\hat{x} - \frac{1}{l}\hat{z}, \quad \vec{b}' = \frac{1}{k}\hat{y} - \frac{1}{l}\hat{z}$$

Obviously $\vec{a}' \cdot \vec{n} = 0$, $\vec{b}' \cdot \vec{n} = 0$

i.e. $\vec{n} \perp a, b$

$\Rightarrow [h\,k\,l] \perp (h\,k\,l)$

(e) in an orthorhombic crystal, $a_1 \neq a_2 \neq a_3$

$$d_{hkl} = \frac{1}{\sqrt{\frac{h^2}{a_1^2} + \frac{k^2}{a_2^2} + \frac{l^2}{a_3^2}}}$$

Problem Set #2 Solutions

Problem 5:

(A) For powder diffraction

$$G = 2k \sin \phi/2$$

$$\text{So } \frac{G}{G_{min}} = \frac{2k/}{2/k} \frac{\sin \phi/2}{\sin \phi/2_{min}} = \frac{\sin \phi/2}{\sin \phi/2_{min}}$$

Compare the successive ratios of $\frac{\sin \phi/2}{\sin \phi/2_{min}}$

for each of A, B and C

with the expected $\frac{G}{G_{min}}$ for each of BCC, FC, C, SC

From attached table. it appears

Crystal A matches SC in reciprocal space

$A \Rightarrow$ SC real space

Crystal B matches FCC in reciprocal space

$B \Rightarrow$ BCC real space

Crystal C matches BCC in reciprocal space

$C \Rightarrow$ FCC in real space.

(B) Lets examine Crystal A the SC more closely

Crystal A is missing a scattering peak at an angle corresponding to $\sin\theta/\lambda = 1/1.73$ implying destructive interference along (1,1

Check:

$$b_1 = 2\pi/a\,\hat{x} \qquad b_2 = 2\pi/a\,\hat{y} \qquad b_3 = 2\pi/a\,\hat{z}$$

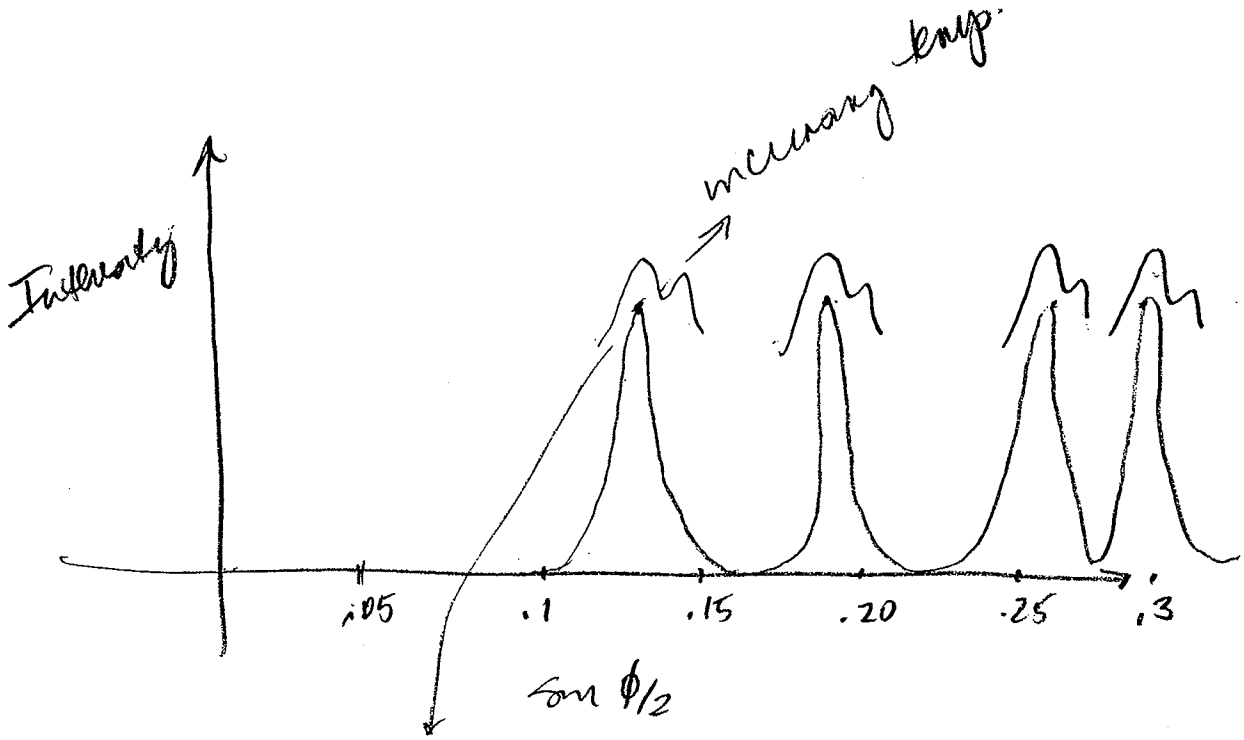
if basis has the same two atoms at $(0,0,0)$ and $(1/2, 1/2, 1/2)$ then

$$S_G = f(1 + e^{-i\,2\pi\left(\frac{h}{2}+\frac{k}{2}+\frac{l}{2}\right)})$$

if $h, k, l = 1, 1, 1$

then $S_G = f(1 + e^{-i\,3\pi}) = 0$

So there is a 2 atom basis for Crystal A. That we may need to pay attention to.



The splitting is not symmetric.

The original peak stays in the same spot with another developing out the side as the crystal continues to distort.

Since {1,0,0} comes from (1,0,0), (0,1,0), (-1,0,0), (0,-1,0) and (0,0), (0,0) distor

the amplitude of undistorted

the 2 peaks will not be equal.

I made my new peaks at higher values of Sin θ/λ but it depends on whether the crystal stretched or contracted. I assumed cont.