3.091 Fall Term 2004

Homework #6

Solutions

From the text:

9-50. $\frac{n}{a^3} = \frac{N_{Av}}{V_{molar}}, \quad V_{molar} = \frac{M_{atomic}}{\rho}$ + solve for *n*, the number of atoms/unit cell.

$$\therefore \quad n = \frac{N_{Av}\rho}{M_{atomic}} \times a^3 = \frac{6.02\times10^{23}\times0.856}{39.0893}\times(5.247\times10^{-8})^3 = 1.90 \cong 2$$

thus, K must be BCC with 2 atoms/unit cell

9-51. $$V_{unit\ cell} = 2\frac{\left(\frac{51.996 \text{ g Cr}}{1 \text{ mol}} \times \frac{1 \text{ mol}}{6.022\times10^{23}}\right)}{7.20\frac{\text{g}}{\text{cm}^3}}$$

$V_{unit\ cell} = a^3 = 2.40 \times 10^{-23}\ \text{cm}^3$

$a = \sqrt[3]{2.40\times10^{-23}\ \text{cm}^3} = 2.88 \times 10^{-8}$ cm

$d^2_{body} = a^2 + a^2 + a^2 = 3a^2$

$d_{body} = \sqrt{3a} = \sqrt{3} \times (2.88 \times 10^{-8}\ \text{cm}) = 5.00 \times 10^{-8}$ cm

$d_{body} = 4\ r_{Cr}$

$$r_{Cr} = \frac{5.00\times10^{-8}\ \text{cm}}{4} = 1.25 \times 10^{-8}\ \text{cm}$$

9-59. From the geometry of the body-centered cubic structure, we find the shortest distance between barium atoms will occur down the body diagonal where

$d_{body} = \sqrt{3}\,a = 4r_{Ba}$

$$r_{Ba} = \frac{\sqrt{3}}{4} \times 0.5025\ \text{nm} \times \frac{1\ \text{m}}{10^9\ \text{nm}} \times \frac{100\ \text{cm}}{1\ \text{m}} = 2.178 \times 10^{-8}\ \text{cm}$$

The shortest distance between barium atoms will be 2 r_{Ba}.
The Ba–Ba distance = 4.356×10^{-8} cm.

Additional questions:

0. in BCC there are 2 atoms / unit cell, so $\frac{2}{a^3} = \frac{N_{Av}}{V_{molar}}$, where $V_{molar} = A/\rho$

(A is atomic mass of iron)

$$\frac{2}{a^3} = \frac{N_{Av} \cdot \rho}{A}$$

$$\therefore \quad a = \left(\frac{2A}{N_{Av} \cdot \rho}\right)^{1/3} = \frac{4}{\sqrt{3}} r$$

$$\therefore \quad r = 1.24 \times 10^{-8}\, cm$$

if we assume that change of phase does not change the radius of the iron atom, then we repeat the calculation in the context of an FCC crystal structure, i.e., 4 atoms per unit cell and $a = 2\sqrt{2}\,r$

$$\rho = \frac{4A}{N_{Av}\,(2\sqrt{2}\,r)^3} = 8.60\, g\, cm^{-3}$$

FCC iron is more closely packed than BCC suggesting that iron contracts upon changing from BCC to FCC. This is consistent with the packing density calculations reported in lecture that give FCC as being 74% dense and BCC 68% dense. The ratio of the densities calculated here is precisely the same:

$$\frac{7.86}{8.60} = \frac{0.68}{0.74}$$

1. First determine the P.D. (packing density) for Au (FCC); then relate it to the molar volume given in the PT.

$$\text{P.D.} = \frac{\text{Vol.Atom/UC}}{\text{Vol.UC}} = \frac{\frac{16\pi r^3}{3}}{a^3} = \frac{16\pi r^3}{3a^3}$$

$$= \frac{16\pi r^3}{3 \times 16\sqrt{2}\, r^3}$$

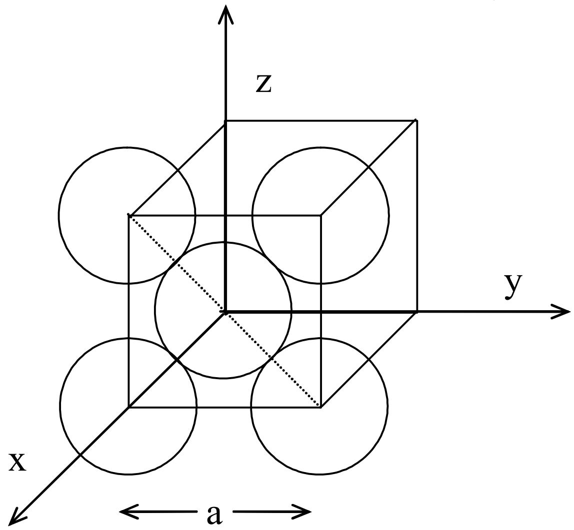
$$\text{P.D.} = \frac{\pi}{3\sqrt{2}} = 0.74 = 74\%$$

Void Volume = 1 – P.D. = 1 – 0.74 = 100% – 74%

From the Packing Density (74%) we recognize the void volume to be 26%. Given the molar volume at 10.3 cm^3/mole, the void volume is:

$0.26 \times 10.3\ cm^3 = 2.68\ cm^3/mole$

2. (a) The answer can be found by looking at a unit cell of Cu (FCC).



Nearest neighbor distance is observed along <110>; second nearest along <100>. The second nearest neighbor distance is found to be "a" (Another way of finding it is looking at LN4, page 12).

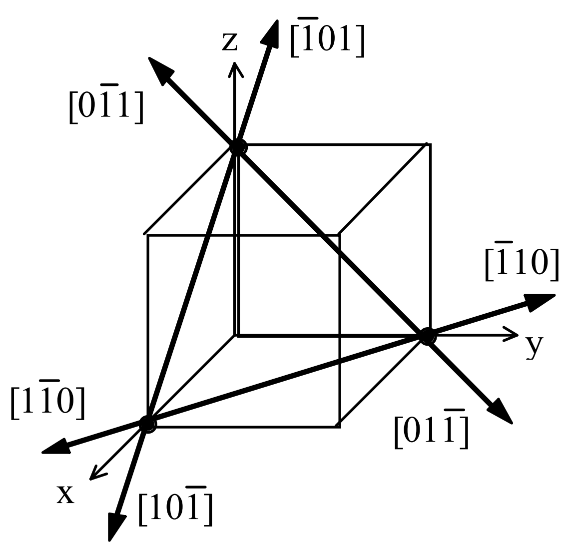
Cu: at. Vol. = 7.1×10^{-6} m^3/mole = $\frac{N}{4} a^3$ (Cu: FCC; 4 at/UC)

$$a = \sqrt[3]{\frac{7.1 \times 10^{-6} \times 4}{6.02 \times 10^{23}}} = \mathbf{3.61 \times 10^{-10}\ m}$$

(b) $d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$

$$d_{110} = \frac{3.61 \times 10^{-10}}{\sqrt{2}} = \mathbf{2.55 \times 10^{-10}\ m}$$

3. Let's look at the unit cell.

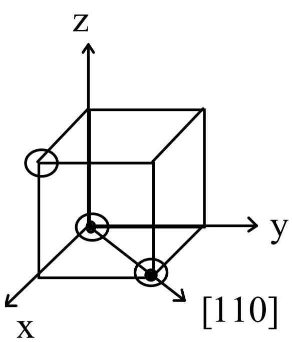


There are six [110]-type directions in the (111) plane. Their indices are:

$$[10\bar{1}]\ [\bar{1}01]\ [\bar{1}10]\ [1\bar{1}0]\ [0\bar{1}1]\ [01\bar{1}]$$

4. Determine the lattice parameter and look at the Unit Cell occupation.
Ba: BCC; at.vol. = 39.24 cm^3/mole; n = 2 atoms/UC

$$3.924 \times 10^{-5}\left(m^3/\text{mole}\right) = \frac{N_A}{2}a^3$$



$$a = \sqrt[3]{\frac{2 \times 3.924 \times 10^{-5}}{6.02 \times 10^{23}}}$$

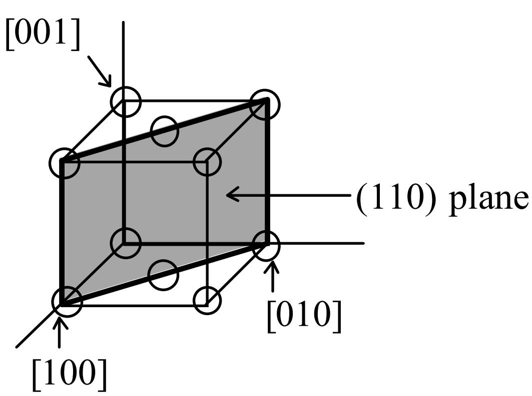
$$a = 5.08 \times 10^{-10}\ m$$

$$\text{linear density} = \frac{1\ \text{atom}}{a\sqrt{2}}$$

$$= \frac{1}{5.08 \times 10^{-10} \times \sqrt{2}}$$

$$\mathbf{= 1.39 \times 10^{9}\ atoms/m}$$

5. Aluminum at 300 K has FCC structure:



Volume unit of a cell:

$$V = \frac{10\ cm^3}{\text{mole}} \times \frac{1\ \text{mole}}{6.02 \times 10^{23}\ \text{atoms}} \times \frac{4\ \text{atoms}}{1\ \text{unit cell}}$$
$$= 6.64 \times 10^{-23}\ cm^3/\text{unit cell}$$

$$V = a^3 \quad \therefore a = \left(6.64 \times 10^{-23}\ \text{cm}^3\right)^{1/3} = 4.05 \times 10^{-8}\ \text{cm}$$

For FCC: $\sqrt{2}a = 4r$; $\therefore$ atomic radius $r = \frac{\sqrt{2}}{4}a = \frac{\sqrt{2}}{4}\left(4.05 \times 10^{-8}\ \text{cm}\right)$
$= \mathbf{1.43 \times 10^{-8}\ cm}$

Planar Packing Fraction of the (110) plane:

area of shadowed plane in above unit cell = $\sqrt{2}a^2$
number of lattice points in the shaded area $= 2\left(\frac{1}{2}\right) + 4\left(\frac{1}{4}\right) = 2$

area occupied by 1 atom = πr^2

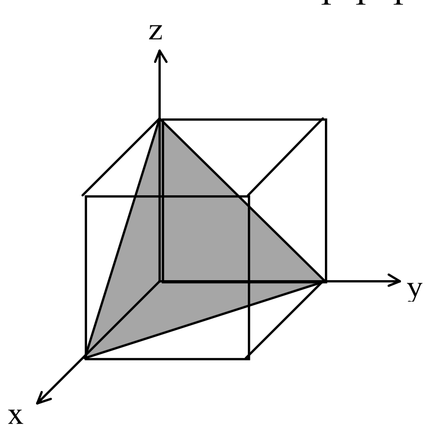
$$\text{Fraction} = \frac{\text{area occupied by atoms}}{\text{total area}} = \frac{2 \cdot \pi r^2}{\sqrt{2}a^2}$$

$$= \frac{2 \cdot \pi\left(1.43 \times 10^{-8}\ \text{cm}\right)^2}{\sqrt{2}\left(4.05 \times 10^{-8}\ \text{cm}\right)^2} = \mathbf{0.554}$$

Linear Packing Density of the [100] direction:

$$\text{Density} = \frac{1\ \text{atom}}{a} = \frac{1\ \text{atom}}{4.05 \times 10^{-8}\ \text{cm}} = 2.47 \times 10^7\ \text{atoms/cm}$$

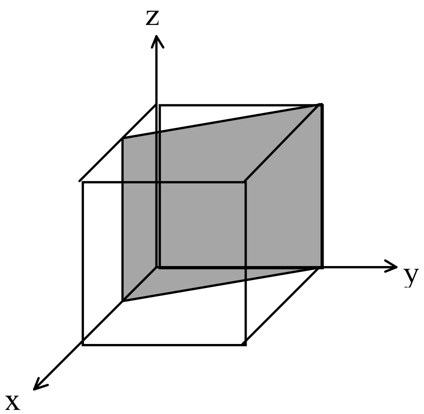
6. (111) inverse = $\frac{1}{1}\ \frac{1}{1}\ \frac{1}{1}$



x = 1, y = 1, z = 1

This plane intersects x axis at x = 1
y axis at y = 1
z axis at z=1

(210) inverse = $\frac{1}{2}\ \frac{1}{1}\ \frac{1}{0}$

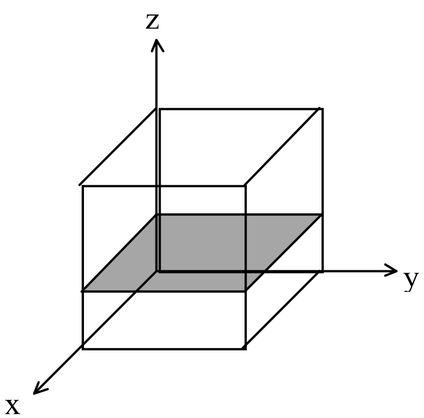


x = 1/2, y = 1, z = infinity

This plane intersects x axis at x = 1/2
y axis at y = 1

This plane does not intersect the z axis.

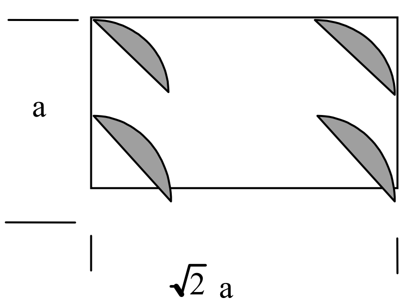
(003) inverse = $\frac{1}{0}\ \frac{1}{0}\ \frac{1}{3}$



x = infinity, y = infinity, z = 1/3

This plane does not intersect either the x or y axis.
This plane intersects the z axis at z = 1/3.

8. (011) looks like this:



$4 \times \frac{1}{4}$ atoms = 1 atom

area = $\sqrt{2}a^2$

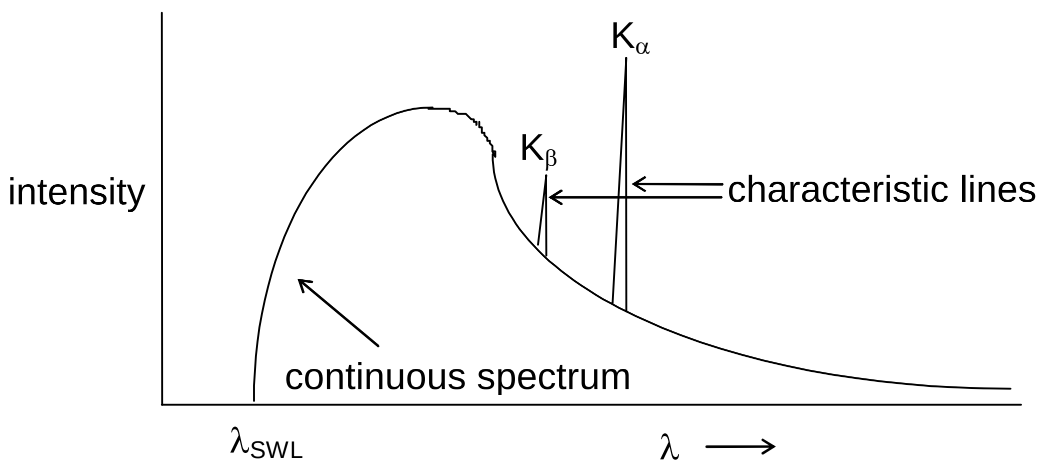
$$\frac{1}{a^3} = \frac{N_{Av}}{V_{molar}} \Rightarrow a = \left(\frac{22.23}{6.02 \times 10^{23}}\right)^{1/3} = 3.33 \times 10^{-8}\,\text{cm}$$

$$\therefore \text{atomic density} = \frac{1}{\sqrt{2}a^2} = 6.376 \times 10^{14}/\text{cm}^2$$

9. A characteristic x-ray spectrum ofCr will show λ_{SWL}, K_β, K_α and the continuous spectrum or *Bremsstrahlung*. We may quantify λ_{K_α} and λ_{SWL}.

$_{24}$Cr:

$$\bar{\nu}_{K_\alpha} = \tfrac{3}{4} R (Z-1)^2 = \tfrac{3}{4} \times 1.097 \times 10^7 (23)^2$$
$$= 4.35 \times 10^9 \text{ m}^{-1}$$
$$\lambda_{K_\alpha} = 2.3 \times 10^{-10} \text{ m}$$
$$\lambda_{SWL} = \frac{hc}{eV} = \frac{1.24 \times 10^{-6} \text{m}}{V} = \frac{1.24 \times 10^{-6} \text{m}}{6 \times 10^4}$$
$$= 2.07 \times 10^{-11} \text{ m}$$



10. (a) $\lambda_{SWL} = \frac{12400}{v} = \frac{12400}{66 \times 10^3} = 0.188$ Å

(b) see sketch above in answer to problem 9. L_α and L_β line will appear to the right of the analogous K lines (at higher values of λ), the L_α to the right of the L_β.

(c) - incident electrons are deflected by negative charge if the electrons of the target

- change in velocity (speed or direction or both) is an acceleration.
- accelerating charge emits radiation.
- extent of acceleration is NOT QUANTIZED.
- spectrum is continuous.