

## LN-4 IDLE MIND SOLUTIONS

1. To do this, the equality of the molar volume

$$\bar{v} = \frac{\# \text{ unit cells}}{\text{mole}} \times \frac{\text{vol}}{\text{unit cell}} = \frac{N_A}{n} \times a^3 \text{ (m}^3\text{/mole)}$$

and

$$\bar{v} = \frac{\text{atomic wt.}}{\text{density}} = \frac{AW \text{ (g/mole)}}{\rho \text{ (g/cm}^3\text{)}}$$

is used, remembering to convert the volume obtained to m<sup>3</sup>/mole using the atomic weight:

$$\frac{AW \text{ (g/mole)}}{\rho \text{ (g/cm}^3\text{)}} \times 10^{-6} \frac{\text{m}^3}{\text{cm}^3} = \frac{N_A \text{ (atoms/mole)}}{n \text{ (atoms/unit cell)}} \times a^3 \text{ (m}^3\text{/unit cell)}$$

Ni: AW = 58.70 g/mole

$$\rho = 8.90 \text{ g/cm}^3$$

FCC, so n = 4 atoms/unit cell

$$a^3 = \frac{(58.70 \text{ g/mole}) (4 \text{ atoms/unit cell})}{(8.90 \text{ g/cm}^3) (6.023 \times 10^{23} \text{ atoms/mole})} \times 10^{-6} \frac{\text{m}^3}{\text{cm}^3}$$

$$= 4.38 \times 10^{-29} \text{ m}^3$$

$$a = (4.38 \times 10^{-29})^{1/3} = \boxed{3.60 \times 10^{-10} \text{ m}}$$

Cr: AW = 52.0 g/mole

$$\rho = 7.19 \text{ g/cm}^3$$

BCC, so n = 2 atoms/unit cell

$$a^3 = \frac{(52.0 \text{ g/mole}) (2 \text{ atoms/unit cell})}{(7.19 \text{ g/cm}^3) (6.023 \times 10^{23} \text{ atoms/mole})} \times 10^{-6} \frac{\text{m}^3}{\text{cm}^3}$$

$$= 2.40 \times 10^{-29} \text{ m}^3$$

$$a = (2.40 \times 10^{-29})^{1/3} = \boxed{2.89 \times 10^{-10} \text{ m}}$$

WATCH OUT!!

$$\rho = \rho$$

2. Mo:  $AW = 95.94 \text{ g/mole}$   
 $\rho = 10.2 \text{ g/cm}^3$   
 BCC, so  $n = 2 \text{ atoms/unit cell}$

$$a^3 = \frac{(95.94 \text{ g/mole}) (2 \text{ atoms/unit cell})}{(10.2 \text{ g/cm}^3) (6.023 \times 10^{23} \text{ atoms/mole})} \times 10^{-6} \frac{\text{m}^3}{\text{cm}^3}$$

$$= 3.12 \times 10^{-29} \text{ m}^3$$

$$a = 3.22 \times 10^{-10} \text{ m}$$

$$\text{For BCC, } a\sqrt{3} = 4r, \text{ so } \boxed{r = 1.39 \times 10^{-10} \text{ m}}$$

3. BCC structure, so  $n = 2$   
 $a = 3.31 \text{ \AA} = 3.31 \times 10^{-10} \text{ m}$   
 $\rho = 16.6 \text{ g/cm}^3$

$$\frac{AW}{\rho} \times 10^{-6} = \frac{N_A}{n} \times a^3$$

$$AW = \frac{(6.023 \times 10^{23} \text{ atoms/mole}) (3.31 \times 10^{-10} \text{ m})^3}{(2 \text{ atoms/unit cell}) (10^{-6} \text{ m}^3/\text{cm}^3)} \times 16.6 \text{ g/cm}^3$$

$$\boxed{= 181.3 \text{ g/mole}}$$

4. Cu is FCC, so:  
 $n = 4$   
 $a = 3.655 \text{ \AA} = 3.655 \times 10^{-10} \text{ m}$   
 $AW = 63.55 \text{ g/mole}$

$$\frac{AW}{\rho} \times 10^{-6} = \frac{N_A}{n} \times a^3$$

$$\rho = \frac{(63.55 \text{ g/mole}) (4 \text{ atoms/unit cell})}{(6.023 \times 10^{23} \text{ atoms/mole}) (3.655 \times 10^{-10} \text{ m})^3} = \boxed{8.64 \text{ g/cm}^3}$$

WATCH OUT!!

$$\rho = \rho$$

5. Ni:  $n = 4$   
 $AW = 58.70 \text{ g/mole}$   
 $\rho = 8.83 \text{ g/cm}^3$

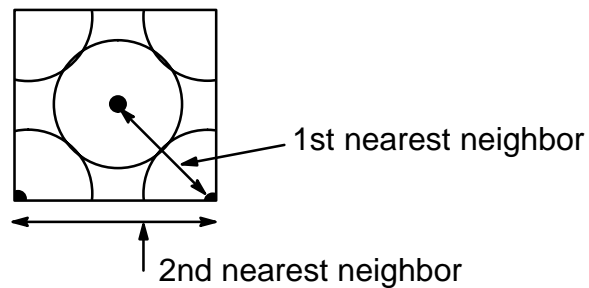
For a face-centered cubic structure, the second nearest neighbor distance equals "a" (see LN4-11).

$$\frac{AW}{\rho} \times 10^{-6} = \frac{N_A}{n} \times a^3$$

$$a^3 = \frac{(58.70 \text{ g/mole}) (10^{-6} \text{ m}^3/\text{cm}^3) (4 \text{ atoms/unit cell})}{(6.023 \times 10^{23} \text{ atoms/mole}) (8.83 \text{ g/cm}^3)}$$

$$= 4.41 \times 10^{-29} \text{ m}^3$$

$$a = 3.61 \times 10^{-10} \text{ m} \times \frac{10^{12} \text{ pm}}{\text{m}} = \boxed{3.61 \times 10^2 \text{ pm}}$$



6. Vanadium:  $AW = 50.94 \text{ g/mole}$   
 $\rho = 5.8 \text{ g/cm}^3$   
 BCC, so  $n = 2$

The highest density would be found in the [111] direction. To find "a":

$$\frac{AW}{\rho} = a^3 \frac{N_A}{n} \rightarrow a^3 = \frac{50.94 \times 2}{5.8 \times 6.023 \times 10^{23}}$$

$$a = 3.08 \times 10^{-8} \text{ cm} = \boxed{3.08 \times 10^{-10} \text{ m}}$$

The length in the [111] direction is  $a\sqrt{3}$ , so there are:

$$2 \text{ atoms}/a\sqrt{3} = 2 \text{ atoms}/(3.08 \times 10^{-10} \times \sqrt{3} \text{ m})$$

$$= \boxed{3.75 \times 10^9 \text{ atoms/m}}$$

WATCH OUT!!

$$\rho = \rho$$

7. This problem can easily be solved by relating it to the unit cell dimensions. (We must watch out for dimensions!)

$$\begin{aligned} \text{BCC, } n &= 2 \\ a &= 3.039 \times 10^{-10} \text{ m} \\ \rho &= 5.81 \text{ g/cm}^3 \end{aligned}$$

$$\frac{\text{At.Wt.}}{\rho} = \text{Mol.Vol.} = \frac{N_A}{n} \times a^3$$

$$\text{At.Wt.} = \frac{N_A}{n} \times a^3 \times \rho$$

$$= \frac{6.02 \times 10^{23}}{2} \times (3.039 \times 10^{-10})^3$$

$$\times 5.81 \left( \frac{\text{at}}{\text{mole}} \times \frac{1}{\text{at/U.C.}} \times \frac{\text{m}^3}{\text{U.C.}} \times \frac{\text{g}}{\text{cm}^3} \right)$$

$$\text{At.Wt.} = \frac{6.02 \times 10^{23}}{2} \times a^3 \times 5.81 \times 10^6 \left( \frac{\text{at}}{\text{mole}} \times \frac{1}{\text{at/U.C.}} \times \frac{\text{m}^3}{\text{U.C.}} \times \frac{\text{g}}{\text{cm}^3} \right)$$

$$\boxed{= 49.1 \text{ g/mole}}$$

appears to be vanadium??

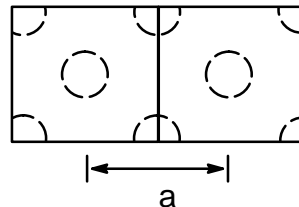
8.  $\text{P.D.} = \frac{\text{Vol. atoms/U.C.}}{\text{Vol./U.C.}}$  for BCC  $\text{P.D.} = \frac{(8\pi r^3)/3}{a^3}$

$$\text{P.D.} = \frac{(8\pi r^3)/3}{(64r^3)/3\sqrt{3}} = \frac{24\sqrt{3}\pi r^3}{3 \times 64r^3} = \frac{\sqrt{3}\pi}{8} = 0.68$$

$$\begin{aligned} a\sqrt{3} &= 4r \\ a &= (4r)/\sqrt{3} \\ a^3 &= (64r^3)/3\sqrt{3} \end{aligned}$$

$$\boxed{\text{P.D.} = 68\%}$$

9. (a) To answer this question we can look at the lecture notes (#4, p. 11) and find for the FCC system (Ni) the second nearest neighbor distance given as  $a$ . Alternately we can look at two adjacent unit cells and confirm " $a$ " to be the distance to the next nearest neighbor. The problem is reduced to the determination of " $a$ ", the lattice constant:



WATCH OUT!!

$$\rho = \rho$$

9. (a) Continued.

$$\frac{\text{At.Wt.}}{\rho} = \frac{58.7}{8.86} = 6.63 \times 10^{-6} \frac{\text{m}^3}{\text{mole}} = \frac{N_A}{4} a^3$$

$$a = \sqrt[3]{\frac{4 \times 6.63 \times 10^{-6}}{6.02 \times 10^{23}}} = \boxed{3.53 \times 10^{-10} \text{ m}}$$

(b) FCC is a close packed structure with **12 nearest neighbors**: six in one plane and three above and below that plane.

10. Au: in the P.T. we find:  
 Structure: FCC  
 At. Vol.:  $10.2 \text{ cm}^3/\text{mole} = 1.02 \times 10^{-5} \text{ m}^3/\text{mole}$

For the FCC system we know that  $a\sqrt{2} = 4r$ . Thus:

$$1.02 \times 10^{-5} = N_A/4 a^3$$

$$a = \sqrt[3]{\frac{4 \times 1.02 \times 10^{-5}}{6.02 \times 10^{23}}} = 4.08 \times 10^{-10} \text{ m}$$

$$a\sqrt{2} = 4r$$

$$r = \frac{4.08 \times 10^{-10} \times \sqrt{2}}{4} = \boxed{1.44 \times 10^{-10} \text{ m}}$$

11. We can solve this problem by considering the effective volume per atom in the two unit cells, BCC and FCC. The volume change in % is then given by  $(V_f - V_i) / V_i \times 100$ . (To simplify calculations, we assume the atomic radius to be unity – 1 Å if you want.)

BCC: 2 at./U.C. 4 (r = unity)	$V_{\text{at.(BCC)}}$  $= 64/6 \sqrt{3}$	$= a^3/2 a \sqrt{3}$  $a^3 = 64/3 \sqrt{3}$	$=$
FCC: 4 at./U.C.	$V_{\text{at.(FCC)}} = a^3/4$ $= (16\sqrt{2})/4$ $= 4\sqrt{2}$	$a = 2\sqrt{2}$ (r = unity) $a^3 = 16\sqrt{2}$	

WATCH OUT!!

$$\rho = \rho$$

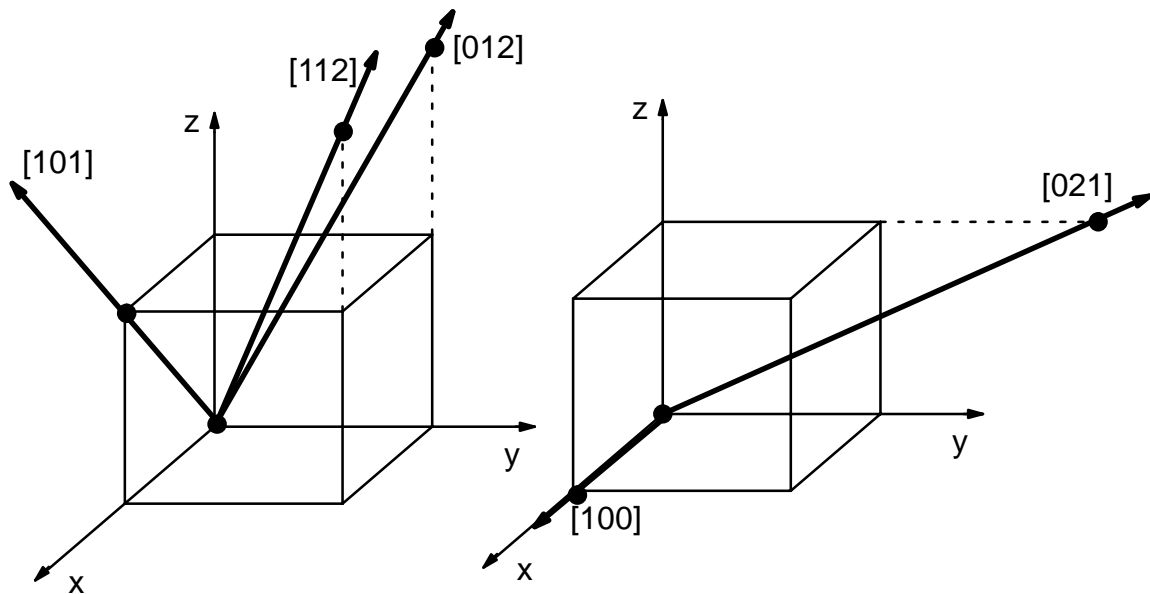
11. Continued.

The volume change for the transformation (in %) is:

$$\Delta V = \frac{V_f - V_i}{V_i} \times 100 = \left[ \frac{\frac{4\sqrt{2}}{64}}{\frac{6\sqrt{3}}{64}} - 1 \right] \times 100 = \left( \frac{24 \times \sqrt{6}}{64} - 1 \right) \times 100$$

$= -8.1\%$

12.

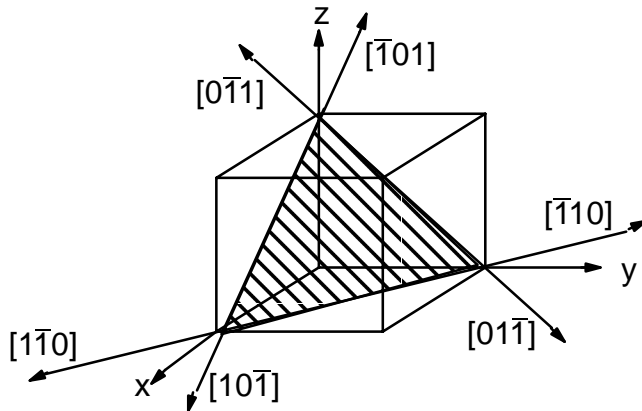


13. (a) The largest “holes” are the “octahedral voids” formed by eight (8) contiguous atoms, for example, about the (very) center of an FCC unit cell. The location of the center:  $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ .
- (b) The total number of octahedral voids per U.C.? One in the center and  $\frac{1}{4}$  void centered on each edge of the U.C. Since there are 12 edges, we have a total of  $(1 + 12/4) = 4$  **octahedral voids**.

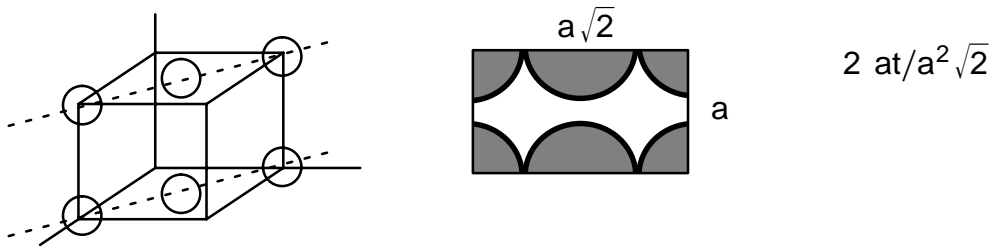
WATCH OUT!!

$$\rho = \rho$$

14. The (111) plane in an FCC structure contains six  $[110]$  directions.



15. We look at the problem on the scale of the U.C. (FCC).



From the P.T. we know:

$$\text{Mol. Vol.} = 9.10 \text{ cm}^3/\text{mole}$$

$$\text{FCC} = 4 \text{ at./U.C.}$$

$$9.1 \times 10^{-6} = N_A/4 a^3$$

$$a = \sqrt[3]{\frac{4 \times 9.1 \times 10^{-6}}{6.02 \times 10^{23}}} = 3.93 \times 10^{-10} \text{ m}$$

$$\frac{2 \text{ atoms}}{a^2 \sqrt{2}} = \frac{2 \text{ atoms}}{\sqrt{2} \times 1.54 \times 10^{-19} \text{ m}^2} = \boxed{9.18 \times 10^{18} \text{ at} \cdot \text{m}^{-2}}$$

WATCH OUT!!

$$\rho = q$$

16. We solve this problem by determining the molar (atomic) volume.

$$\text{Mol. Vol.} = \text{at. Wt.} / \rho = N_A / 2a^3$$

We need to know "a" – given  $d_{(110)}$

$$d_{(110)} = \frac{a}{\sqrt{2}}$$

$$a = \sqrt{2} \times 2.04 \times 10^{-10} \text{ m} = 2.89 \times 10^{-10} \text{ m}$$

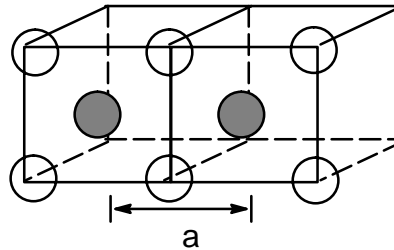
$$\text{Mol. Vol.} = \frac{6.02 \times 10^{23}}{2} \times (2.89 \times 10^{-10})^3 = 7.26 \text{ cm}^3/\text{mole}$$

$$\text{Mol. Vol.} - \frac{\text{At. Wt.}}{\rho} = 7.26$$

$$\text{At. Wt.} = 7.26 \times 7.21 \left[ \frac{\cancel{\text{cm}^3}}{\text{mole}} \times \frac{\text{g}}{\cancel{\text{cm}^3}} \right] = \boxed{52.3}$$

17. Pt: A look at the U.C.:

The face centered atoms are next nearest neighbors! They are spaced at "a".

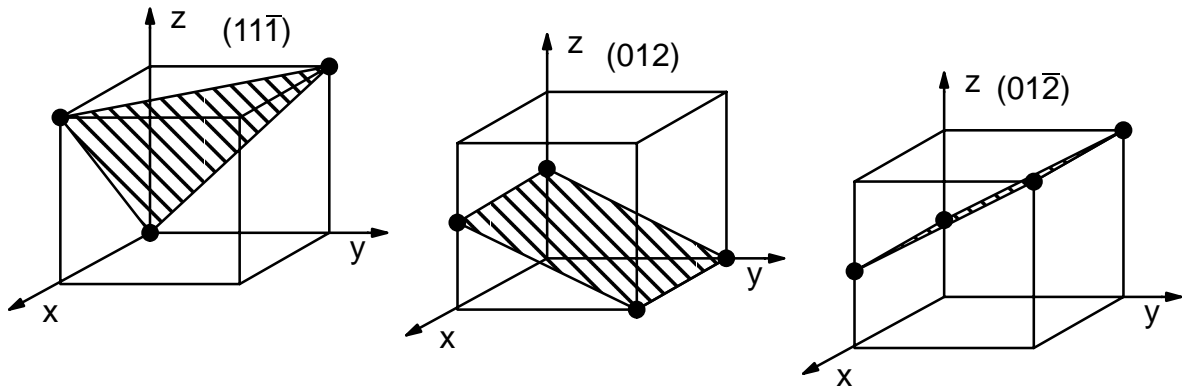


"a", the lattice constant, can be found to be  $3.93 \times 10^{-10} \text{ m}$ .

WATCH OUT!!

$$\rho = \rho$$

18.



19. In nature most solids appear as polycrystalline systems, which consist of interwoven conglomerates of small crystallites (grains with diameters ranging from  $<10^{-6}$  to  $>10^{-4}$  m). Anisotropy in materials is contingent on the existence of order over macroscopic dimension. Thus "single crystals" will exhibit properties that are dependent on direction (anisotropy). Polycrystalline materials, on the other hand, appear isotropic because of the random spatial orientation of the crystallites.

20. Required: BCC  $\rightarrow$  2 atoms/u.c.

$$\text{Molar Volume} = \frac{\text{Atomic Weight}}{\rho} = \frac{N_A}{2} \times a^3$$

$$\text{Atomic Weight} = 3.01 \times 10^{23} \times (3.039 \times 10^{-10})^3 \times \frac{5.81}{10^{-6}}$$

At.Wt. = 49.1
---------------

WATCH OUT!!

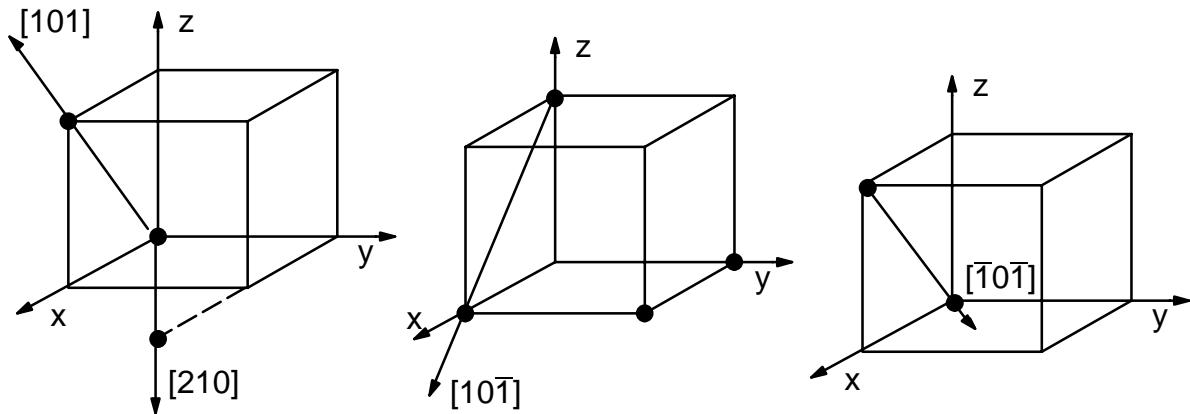
$$\rho = \rho$$

21. Required: SC  $\rightarrow$  1 atom/u.c.  
 $a = 2r$

$$\text{Packing Density} = \frac{\text{Volume of Atoms/Unit Cell}}{\text{Volume/Unit Cell}}$$

$$= \frac{4\pi \frac{r^3}{3}}{a^3} = \frac{4\pi r^3}{8r^3} = \frac{\pi}{6} = \boxed{0.524 = 52.4\%}$$

22.



23. Required: FCC = 4 atoms/u.c.  
 $d_{(hkl)} = a / \sqrt{h^2 + k^2 + l^2}$

$$\frac{\text{Atomic Weight}}{\text{Density}} = \text{Molecular Volume} = a^3 \frac{N_A}{4} \quad (a = d_{(111)} \sqrt{3})$$

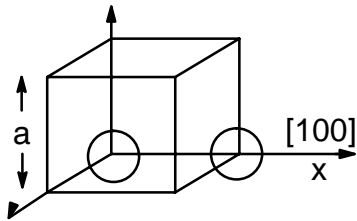
$$= 3d^3 \sqrt{3} \frac{N_A}{4}$$

$$\text{Atomic Weight} = 3 \times (2.08 \times 10^{-10})^3 \sqrt{3} \frac{6.02 \times 10^{23}}{4} \times \frac{8.96}{10^{-6}} = \boxed{63.1}$$

WATCH OUT!!

$$\rho = \rho$$

24. It is most convenient to resort to the Unit Cell dimensions:



We recognize that there is one atom per lattice constant ( $a$ ) in the  $[100]$  direction

From the P.T.: At.Wt. = 106.4  
 $\rho = 12.0 \text{ g/cm}^3$   
 Structure = FCC

$$\frac{106.4}{12.0} = a^3 \frac{N_A}{4}$$

$$a = \sqrt[3]{\frac{106.4 \times 4}{12.0 \times N_A}} = 3.89 \times 10^{-8} \text{ cm}$$

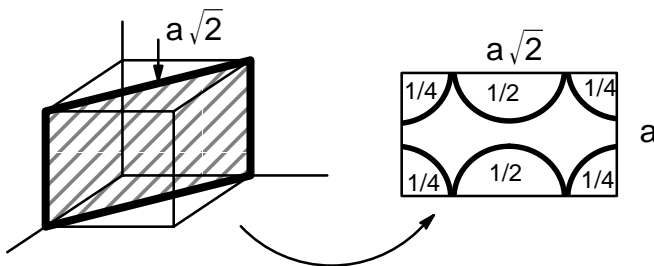
(We used  $\rho$  in units of  $\text{g/cm}^3$ .)

$$= 3.89 \times 10^{-10} \text{ m}$$

We have one atom/ $(3.89 \times 10^{-10} \text{ m})$ , or:

**$2.57 \times 10^9 \text{ atoms/m}$  in the  $[100]$  direction.**

- 25.



We recognize two atoms within the area  $a^2 \sqrt{2}$ .

Cu: At.Wt. = 63.546  
 $\rho = 8.96 \text{ g/cm}^3$   
 Structure = FCC

$$\frac{63.546}{8.96} = a^3 \frac{N_A}{4}$$

$$a = \left( \frac{4 \times 63.546}{8.96 \times N_A} \right)^{1/3} = 3.62 \times 10^{-8} \text{ cm} = \boxed{3.61 \times 10^{-10} \text{ m}}$$

$$2 \text{ atoms} / \left[ \sqrt{2} \times (3.62 \times 10^{-10})^2 \right] = \boxed{1.08 \times 10^{19} \text{ atoms/m}^2}$$

WATCH OUT!!

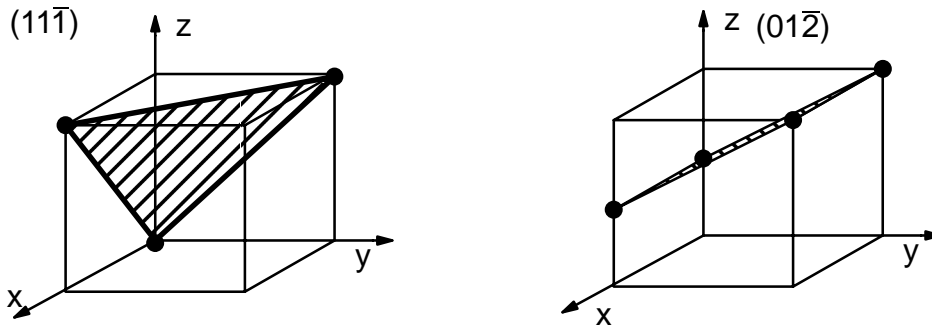
$$\rho = \rho$$

26. In the simple cubic system the void at the center of the unit cell is bounded by the eight (8) corner atoms. The diameter of an interstitial atom is therefore given by the body diagonal minus  $2r$ .

$$D = a\sqrt{3} - 2r = 2r\sqrt{3} - 2r = 2r(\sqrt{3} - 1)$$

$$R_{(\text{interstitial})} = r(\sqrt{3} - 1) = 0.732 r$$

27.



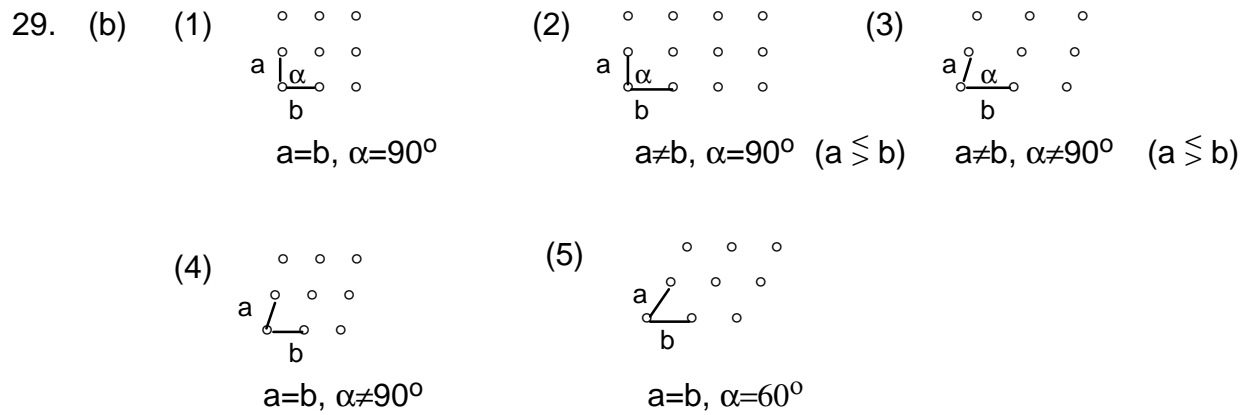
28. Diffraction experiments show us that Cu has an FCC crystal structure. This is not a primitive unit cell.  $\{111\}$  planes are found (by inspection of the FCC unit cell) to have the widest spacing.  $\{100\}$  and  $\{110\}$  planes are not the widest spaced planes because the additional lattice sites in the FCC structure occupy positions between these planes.

29. (a) There are five ways in which points can be arranged in two dimensions so that every point has identical surroundings. The square lattice includes squares of all sizes and orientation. We can also obtain such a lattice distribution by operating with a rectangular pattern. By changing to axes at some random angle ( $\alpha$ ), we obtain two additional arrangements: a rhombus (deduced from a square) and a parallelepiped (deduced from a rectangle). The fifth pattern is a rhombus for which  $\alpha = 60^\circ$  (a triangular pattern).

(continued)

WATCH OUT!!

$$\rho = \rho$$



30. Fe at room temperature is BCC (body centered cubic); taking the atomic radius of Fe as  $1.26 \text{ \AA}$ , we have a face of the unit cell (with  $a\sqrt{3} = 4r$ ) at:

$$a^2 = \frac{16r^2}{3} = (8.47 \text{ \AA})^2 = 8.47 \times 10^{-20} \text{ m}^2$$

The face (100) of the unit cell contains 1 atom ( $4 \times 1/4$  atoms). We therefore have:

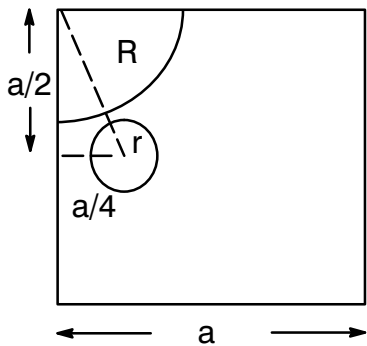
$$\frac{1 \text{ atom}}{8.47 \times 10^{-20} \text{ m}^2} = \frac{1 \text{ atom}}{8.47 \times 10^{-14} \text{ mm}^2}$$

or:  $\boxed{1.12 \times 10^{13} \text{ atoms/mm}^2}$

WATCH OUT!!

$$\rho = \rho$$

31. In the BCC structure of vanadium, the largest void can readily be identified as located about the site  $1/2, 1/4, 0$  in the unit cell. (There obviously are a large number of such equivalent sites in each unit cell.)



Look at a unit cell face for V with radius ( $R$ ); the distance of the site from the origin ( $0$ ) is, according to Pythagoras:

$$(R + r)^2 = \left(\frac{a}{2}\right)^2 + \left(\frac{a}{4}\right)^2 \text{ and}$$

$$(R + r) = \sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{a}{4}\right)^2} = \frac{a}{4}\sqrt{5}$$

$$r = \frac{a}{4}\sqrt{5} - R$$

But:  $a = \frac{4R}{\sqrt{3}}$  (BCC) and  $\frac{4R\sqrt{5}}{\sqrt{3} \times 4} - R = r$        $\frac{R\sqrt{5}}{\sqrt{3}} - R = r$

or:  $r = R\left(\frac{\sqrt{5}}{\sqrt{3}} - 1\right)$

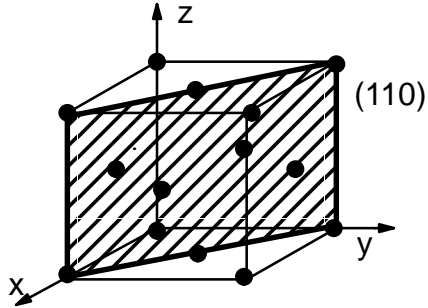
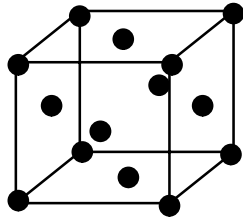
$R$  for vanadium =  $1.34\text{\AA}$

$$r = 1.34 \left(\frac{\sqrt{5}}{\sqrt{3}} - 1\right) = 0.39\text{\AA} = 3.9 \times 10^{-11} \text{ m}$$

WATCH OUT!!

$\rho = \rho$

32.



- (a) atoms/unit cell:  $(8 \times 1/8) + (6 \times 1/2) = 4 \text{ atoms/u.c.}$
- (b) See above.
- (c) The intercepts of a plane (421) on the x and y coordinates are the reciprocals  $1/4$  and  $1/2$ ; thus the ratio of the intercepts is  $1/2$ .
- (d) The atomic packing factor:  $P.D. = \frac{\text{vol. atoms/u.c.}}{\text{vol./u.c.}}$   
 For BCC lattices we have 2 atoms/u.c..

$$a\sqrt{3} = 4r \quad \text{or} \quad a = \frac{4r}{\sqrt{3}} \quad \text{and} \quad a^3 = \frac{64r^3}{3\sqrt{3}}$$

Thus:

$$P.D. = \frac{\frac{8\pi r^3}{3}}{\frac{64r^3}{3\sqrt{3}}} = \frac{24\sqrt{3}\pi r^3}{3 \times 64r^3} = \frac{\pi\sqrt{3}}{8} = \boxed{0.68 = 68\%}$$

33. Determine the linear density of atoms/cm along the [110] direction in Cu. The simplest approach involves the unit cell dimensions:

Cu: FCC (4 atoms/u.c.)

$\langle 110 \rangle$  are face-diagonals

$$a\sqrt{2} = 4r, \text{ or } 2 \text{ atoms}/a\sqrt{2}$$

The calculation requires knowledge of "a", the lattice constant:

$$7.1 \times 10^{-6} = N_A/4 a^3$$

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

WATCH OUT!!

$$\rho = \rho$$

33. Continued.

Accordingly:

$$\frac{2 \text{ atoms}}{3.61 \times 10^{-10} \times \sqrt{2} \text{ m}} \times \frac{1 \text{ m}}{100 \text{ cm}} = \boxed{3.9 \times 10^7 \text{ atoms/cm along } \langle 110 \rangle}$$

34. Determine the planar atomic density per  $\text{m}^2$  for Ni (FCC) in  $\{111\}$  planes.  
In the unit cell we find  $(3 \times 1/2) + (3 \times 1/6)$  atoms = 2 atoms  
within the area of the  $\{111\}$  planes.

First we determine "a", the lattice constant:

$$6.59 \times 10^{-6} = \frac{N_A}{4} \times a^3 ; a = \sqrt[3]{\frac{4 \times 6.59 \times 10^{-6}}{6.02 \times 10^{23}}} = 3.52 \times 10^{-10} \text{ m}$$

Area of equilateral triangle:

$$A = h \times (a\sqrt{2})/2 = h \times (a/\sqrt{2})$$

$$h^2 = (a\sqrt{2})^2 - \left(\frac{a}{\sqrt{2}}\right)^2 = 2a^2 - \frac{a^2}{2} = \frac{3}{2} a^2$$

$$h = \sqrt{\frac{3}{2}} a$$

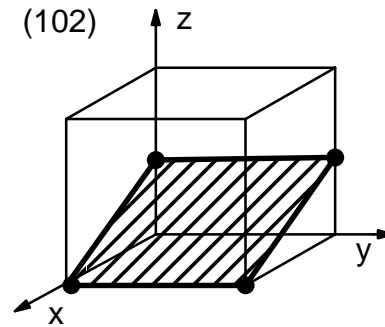
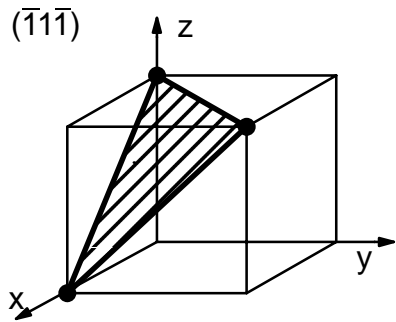
$$A = \sqrt{\frac{3}{2}} a \times \frac{a}{\sqrt{2}} = \frac{\sqrt{3}a^2}{2} = 1.07 \times 10^{-19} \text{ m}^2$$

$$\text{Planar Atomic Density} = \frac{2 \text{ atoms}}{1.07 \times 10^{-19} \text{ m}^2} = \boxed{1.86 \times 10^{19} \text{ Ni atoms/m}^2}$$

WATCH OUT!!

$$\rho = \rho$$

35.



$$36. \quad a = (2.02\text{\AA})\sqrt{2} = 2.86\text{\AA} = 2.86 \times 10^{-10} \text{ m}$$

$n = 2$  for the BCC structure

$$\rho = 7.87 \text{ g/cm}^3 = 7.87 \times 10^6 \text{ g/m}^3$$

$$\text{A.W.} = \left(\frac{N_A}{n}\right)a^3\rho = \frac{6.023 \times 10^{23} \text{ atoms/mol}}{2 \text{ atoms/unit cell}} (2.86 \times 10^{-10} \text{ m})^3 7.87 \times 10^6 \text{ g/m}^3$$

$$= \boxed{55.44 \text{ g/mol}}$$

37. (a) To find the Miller indices of  $\infty, 2, \bar{1}$ , take the reciprocal:

$$\frac{1}{\infty} \quad \frac{1}{2} \quad \frac{1}{-1}$$

Multiply by 2 so that they are all integers:  $0 \quad 1 \quad \bar{2}$

Put parenthesis around them: **(012)**

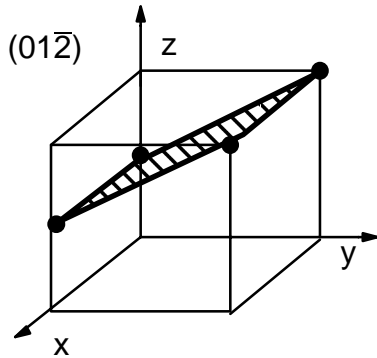
(continued)

WATCH OUT!!

$$\rho = \rho$$

37. Continued.

(b)



(c) In the cubic system, the indices of directions normal to a plane are given by the Miller indices of the plane: **[012]**

38. This is the same problem as #6 of this lecture note!

39. We know:

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

$$\sqrt{h^2 + k^2 + l^2} = \frac{a}{d_{(hkl)}} = \frac{3.524}{1.246} = 2.828$$

$$h^2 + k^2 + l^2 = 8 = (2^2 + 2^2 + 0)$$

**The family of planes is {220}.**

40. FCC; determine the molar volume and relate to the # uc's; getting, a, the lattice constant permits determination of r ( $a\sqrt{2} = 4r$ )

$$\text{molar volume} = 195.09 \frac{\text{g}}{\text{mole}} \times \frac{1\text{cm}^3}{21.4\text{g}} = \frac{9.12\text{cm}^3}{\text{mole}} \times \frac{1\text{m}^3}{10^6\text{cm}^3} = \frac{N_A}{4} \times a^3$$

$$a = \sqrt[3]{\frac{9.12 \times 10^{-6} \times 4}{6.02 \times 10^{23}}}$$

$$a = 3.93 \times 10^{-10}\text{m}$$

$$a\sqrt{2} = 4r$$

$$r = \frac{a\sqrt{2}}{4} = \frac{3.93 \times 10^{-10} \times \sqrt{2}}{4}$$

$$r = \boxed{1.39 \times 10^{-10}\text{m}}$$

WATCH OUT!!

$$\rho = \rho$$

41. Determine the atomic radius to get the Vol atoms/mole and subtract that from the molar volume. Alternately, we may determine the packing density and use that (determined in school as 74%) to get the void volume (26% of the molar volume). To make the solution simpler, I would use the data from the previous question.

$$\text{From above } 9.12 \text{ cm}^3/\text{mole} \times (1 - 0.74) = \boxed{2.37 \text{ cm}^3/\text{mole void volume}}$$

$$\text{or } \left(\frac{N}{4} \times a^3\right) - N \times \frac{4\pi r^3}{3} = \text{void volume/ mole}$$

$$\frac{6.02 \times 10^{23}}{4} \times (3.92 \times 10^{-10})^3 - 6.02 \times 10^{23} \times \frac{4\pi \times (1.39 \times 10^{-10})^3}{3}$$

$$9.07 \times 10^{-6} - 6.77 \times 10^{-6} = \boxed{2.35 \text{ cm}^3/\text{mole}}$$

42. I would go and read the lecture notes! (LN4, page 1). Accordingly, I would put some Ge into a quartz glass, heat it up to above the melting point – just a bit so that all is molten ( I would have to do that in an inert gas, otherwise, that Ge would be oxidized in air  $\text{Ge} + \text{O}_2 \rightarrow \text{GeO}_2$ ,  $\text{GeO}_2 + \text{Ge} \rightarrow 2 \text{GeO} \uparrow$  the final compound is volatile and escapes – all that would happen: a lot of smoke is generated and there would be no Ge left to melt). I would extract heat somehow from the bottom until all the melt is cooled to below the melting point and then I would pray that only a single crystal was formed in the process.

43. Self explanatory: I hope you did it!

44. The simplest way to differentiate the 2 samples is to put them into a dissolving solution (dilute nitric acid, HF and the like, could do it – you do not have to know this). On the single crystal sphere you would notice etch pits with distinct symmetry features which reflect internal atomic order; there would be no geometric patterns on the surface of the etched glass sphere. You could also take a hammer and smash the sample – expect on the glass, a typical conchoidal fracture – on the crystal appearance of some facets – flat areas reflecting exposure of low index planes.

45.  $\{110\} = (110), (\bar{1}10), (10\bar{1}), (\bar{1}\bar{1}0)$   
 $(101), (1\bar{1}0), (0\bar{1}1), (\bar{1}0\bar{1})$   
 $(011), (\bar{1}01), (01\bar{1}), (0\bar{1}\bar{1})$   
 (see lecture notes)

WATCH OUT!!

$$\rho = \rho$$

46.  $\langle 100 \rangle$  linear density =  $\frac{2 \cdot \frac{1}{2} \text{ atoms}}{a} = \frac{1 \text{ atom}}{a}$

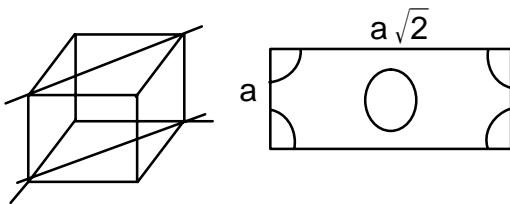
[Sr: FCC;  $n=4$  At.wt = 87.62;  $\rho = 2.6 \text{ g/cm}^3$ ]

$$\text{mol vol} = \frac{\text{At.wt}}{\rho} = \frac{N}{4} a^3$$

$$a = \sqrt[3]{\frac{4 \cdot \text{At.wt}}{\rho \cdot N}} = \sqrt[3]{\frac{4 \cdot 87.62}{2.6 \cdot 6.02 \cdot 10^{23}}} = 6.07 \cdot 10^{-8} \text{ cm} \times \frac{1 \text{ m}}{100 \text{ cm}}$$

$$\text{linear density} = \frac{1 \text{ atom}}{6.07 \cdot 10^{-10} \text{ m}} = \boxed{1.65 \times 10^9 \text{ atoms/m}}$$

47. Ta: BCC;  $n=2$ ; At.wt. = 180.95;  $\rho = 16.6 \text{ g/cm}^3$

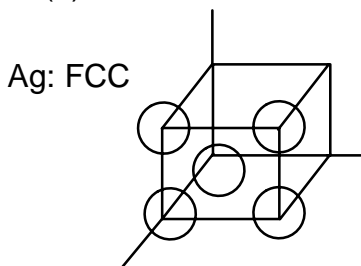


$$\text{planar density} = 2 \text{ atoms}/a^2 \sqrt{2}$$

$$\text{at. vol} = \frac{180.95}{16.6} = \frac{N}{2} a^3 \quad ; \quad a = \sqrt[3]{\frac{10.9 \cdot 10^{-6} \cdot 2}{6.02 \cdot 10^{23}}} = 3.31 \times 10^{-10} \text{ m}$$

$$\text{planar atom density} = \frac{2 \text{ atoms}}{a^2 \sqrt{2}} = \frac{2 \text{ atoms}}{\sqrt{2} \cdot (3.31 \cdot 10^{-10} \text{ m})^2} = \boxed{1.29 \times 10^{19} / \text{m}^2}$$

48. (a)



nearest neighbors are along

$$a\sqrt{2} \text{ at } a\sqrt{2}/2 \quad ;$$

second nearest neighbors are spaced at "a".

$$\text{molar volume} = \frac{\text{At.wt}}{\rho} = \frac{N}{4} a^3 \quad ; \quad a = \sqrt[3]{\frac{\text{at.wt} \cdot 4}{\rho \cdot N}} = \sqrt[3]{\frac{107.87 \cdot 10^{-6} \cdot 4}{10.5 \cdot 6.02 \cdot 10^{23}}}$$

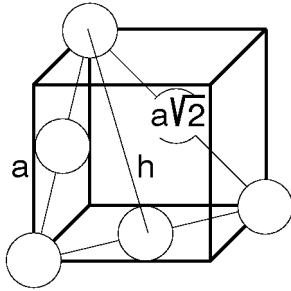
$$a = \boxed{4.09 \times 10^{-10} \text{ m}} = \text{next nearest neighbor or distance}$$

$$(b) \quad d_{\{110\}} \text{ Ag: } \frac{a}{\sqrt{1^2 + 1^2 + 0^2}} = \frac{a}{\sqrt{2}} = \frac{4.09 \cdot 10^{-10}}{\sqrt{2}} = \boxed{2.89 \times 10^{-10} \text{ m}}$$

WATCH OUT!!

$$\rho = \rho$$

49.



$$\text{planar density in } \{111\} = \frac{2 \text{ atoms}}{\frac{a\sqrt{2}}{2}} \cdot h$$

$$h^2 = (a\sqrt{2})^2 - \left(\frac{a\sqrt{2}}{2}\right)^2$$

$$= 2a^2 - \frac{a^2}{2} = \frac{3}{2}a^2$$

$$h = a\sqrt{\frac{3}{2}}$$

$$\text{planar atom density} = \frac{2 \text{ atoms}}{\frac{a\sqrt{2}}{2}} \cdot \frac{1}{a\sqrt{\frac{3}{2}}} = \frac{2 \text{ atoms}}{a^2 \sqrt{3}/2} \text{ m}^{-2}$$

$$= \frac{2 \text{ atoms}}{a^2 \sqrt{3}/2} \text{ m}^{-2}$$

$$= \boxed{7.47 \times 10^{18} \text{ atoms/m}^2}$$

WATCH OUT!!

 $\rho = \rho$

