1.1 A jet turbine rotates at a velocity or 7,500 rpm. Calculate the stress acting on the turbine blades if the turbine disc radius is 70 cm and the cross-sectional area is 15 cm^2. Take the length to be 10 cm and the alloy density to be 8.5 gcm^{-3}.

Mass, m = ρv = 8.5 x 10 x 15 = 1275 g

= 1.275 kg

Centripetal acceleration, $a_c = w^2 r_{disc}$

$$= \left(7500 \frac{1}{60} 2\pi\right)^2 x\, 0.7$$

$$= 0.43 \text{ x } 10^6 \text{ ms}^{-2}$$

$$\text{Stress } \sigma = \frac{F}{A} = \frac{ma}{A} = \frac{1.275\, x\, 0.43\, x\, 10^6}{15\, x\, 10^{-4}}$$

$$\sigma = 367\ MPa$$

1.2 The material of the jet turbine blade in Problem 1.1, Superalloy IN 718, has a room-temperature yield strength equal to 1.2 GPa; it decreases with temperature as

$\sigma = \sigma_0\,[1 - (T - T_0)/(T_m - T_0]$,

where T_0 is the room temperature and T_m is the melting temperature in K (T_m = 1,700 K). At what temperature will the turbine flow plastically under the influence of centripetal forces?

$T_m = 1700$ K $\qquad \sigma_0 = 1.2$ GPa

$T_0 = 298$ K $\qquad \sigma = 367$ MPa

$$\sigma = \sigma_0\left(1 - \frac{T - T_0}{T_m - T_0}\right)$$

$$1 - \frac{\sigma}{\sigma_0} = \frac{T - T_0}{T_m - T_0}$$

$$(T_m - T_0)\left(1 - \frac{\sigma}{\sigma_0}\right) = T - T_0$$

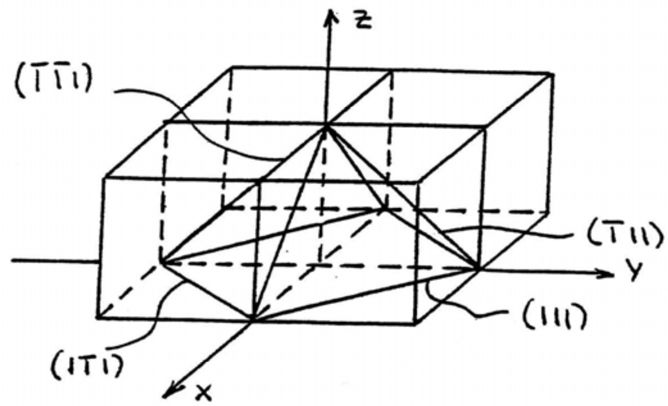
$$T = (T_m - T_0)\left(1 - \frac{\sigma}{\sigma_0}\right) + T_0$$

$$= (1700 - 298)\left(1 - \frac{367 \cdot 10^6}{1.2 \cdot 10^9}\right) + 298$$

$$= 1271 \text{ K}$$

$$\boxed{T = 1271 \text{ K}}$$

1.4 On eight cubes that have one common vertex, corresponding to the origin of axes, draw the family of *{111}* planes. Show that they form an octahedron and indicate all <110> directions.



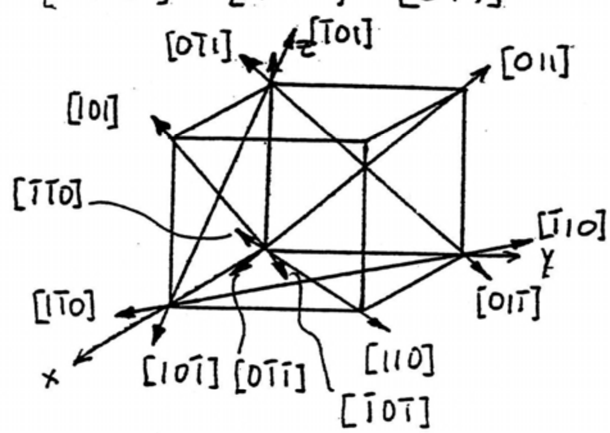
In order to get an octahedron, the above figure contained in the four cubes must be repeated in −z direction.

$\langle 110 \rangle$ = $[110]$ $[101]$ $[011]$

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

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

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



1.5 The frequency of loading is an important parameter in fatigue. Estimate the frequency of loading (in cycles per second, or Hz) of an automobile tire in the radial direction when the car speed is 100km/h and the wheel diameter is 0.5 m.

1 cycle = $2\pi r = 2\pi \text{ x } 0.25$ m

$$\text{Frequency, } \nu = \frac{speed}{cycle} = \frac{100kmh^{-1}}{2\pi \ x \ 0.25}$$

$$= \frac{100 \ x \ 10^3}{0.5\pi} h^{-1}$$

$$\nu \ = \ 17.68 \text{ Hz}$$

1.6 Indicate, by their, indices and in a drawing, six directions of the <112> family.

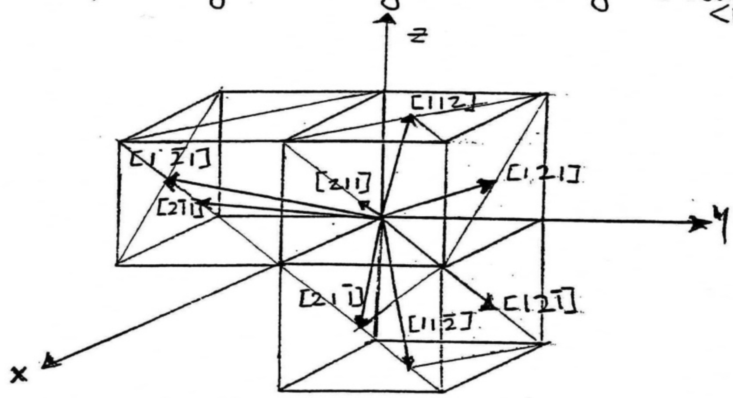
<1 1 2> ⇒

[1 1 2] [$\bar{1}$ 1 2] [1 $\bar{1}$ 2] [1 1 $\bar{2}$] [$\bar{1}$ $\bar{1}$ 2] [$\bar{1}$ 1 $\bar{2}$] [1 $\bar{1}$ $\bar{2}$]

[1 2 1] [$\bar{1}$ 2 1] [1 $\bar{2}$ 1] [1 2 $\bar{1}$] [$\bar{1}$ $\bar{2}$ 1] [$\bar{1}$ 2 $\bar{1}$] [1 $\bar{2}$ $\bar{1}$]

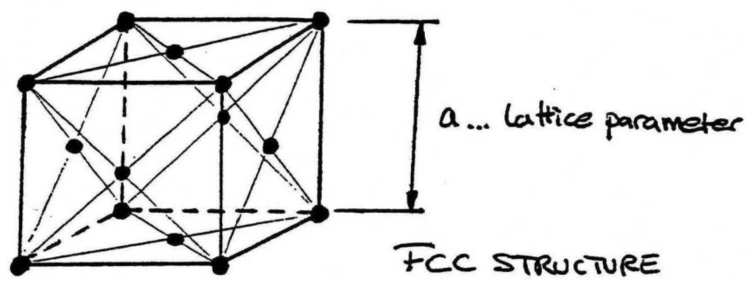
[2 1 1] [$\bar{2}$ 1 1] [2 $\bar{1}$ 1] [2 1 $\bar{1}$] [$\bar{2}$ $\bar{1}$ 1] [$\bar{2}$ 1 $\bar{1}$] [2 $\bar{1}$ 1]

The following drawing shows 8 of the directions in <112> famil



1.7 The density of Cu is 8.9 g/cm^3 and its atomic weight (or mass) is 63.546. It has the FCC structure. Determine the lattice parameter and the radius of atoms**.**

<u>Given</u> $\rho = 8.9\ g/cm^3$ $M = 63.546\ g$



Lattice parameter:

1 unit cubic cell contains $\left(8\cdot\frac{1}{8}+6\cdot\frac{1}{2}\right) = 4$ atoms $= N$

$$\rho = \frac{N\cdot M}{a^3\cdot N_A}$$ where N_A ... Avogadro's number ($6.02\cdot10^{23}$ atoms)

$$a = \sqrt[3]{\frac{N\cdot M}{\rho\cdot N_A}} = \sqrt[3]{\frac{4\ atoms\cdot 63.546\ g}{8.9\ g/cm^3\cdot 6.02\cdot10^{23}\ atoms}} = 0.362\ nm$$

Radius of atoms:

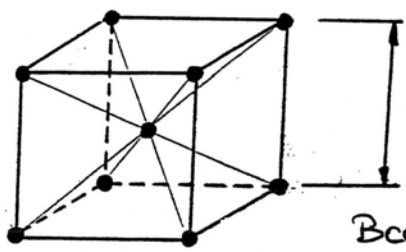
Diagonal of the face of the cube : $\sqrt{2}a = 4\cdot r_{Cu}$

$$r_{Cu} = \frac{\sqrt{2}}{4}a = \frac{\sqrt{2}}{4}\cdot 0.362\cdot10^{-9}\ m = 0.128\ nm$$

$$\boxed{a = 0.362\ nm \text{ and } r_{Cu} = 0.128\ nm}$$

1.8 The lattice parameter for W(BCC) is a = 0.32 nm. Calculate the density, knowing that the atomic weight (or mass) of W is 183.85.

Given $a = 0.32$ nm $M = 183.85$ g



The cubic unit cell contains $\left(8 \cdot \frac{1}{8} + 1\right) = 2$ atoms $= N$

Density : $\rho = \frac{\text{mass}}{\text{volume}}$

$$\rho = \frac{M \cdot N}{a^3 \cdot N_A}$$ where N_A... Avogadro's number ($6.02 \cdot 10^{23}$ atoms)

$$= \frac{183.85\,\text{g} \cdot 2\,\text{atoms}}{(0.32 \cdot 10^{-7}\,\text{cm})^3 \cdot 6.02 \cdot 10^{23}\,\text{atoms}} = 18.64\ \text{g/cm}^3$$

$$\boxed{\rho_W = 18.64\ \text{g/cm}^3}$$

1.10 MgO has the same structure as NaCl. If the radi of O^{2-} and Mg^{2+} ions are 0.14 nm and 0.070 nm, respectively, determine (a) the packing factor and (b) the density of the material. The atomic weight of O_2 is 16 and that of Mg is 24.3.

$a = 2r_{Mg}{}^{2+} + 2r_O{}^{2-}$

Given: $r_{Mg\ 2+} = 0.07$ nm and $r_{O\ 2-} = 0.140$ nm

a = 0.420 nm

$V_{unit\ cell} = a^3 = (0.420nm)^3 = 0.0741nm\ ^3$

There are 4 Mg^{2+} ions and 4 O^{2-} ions per cell, giving a total ionic volume of

$4x\ 4/3\ \pi r^3{}_{Mg}{}^{2+} + 4\ x\ 4/3\ \pi r^3{}_O{}^{2-}$

$= (16\pi/3)\ [(0.07)^3 + 0.014^3]\ nm^3$

$= 0.0517\ nm^3$

Therefore, the packing factor = 0.0517/0.0741 = 0.698

1.11 Germanium has the diamond cubic structure with interatomic spacing of 0.245 nm. Calculate the packing factor and density. (The atomic weight of germanium is 72.6.)

a = 0.245 nm

$V_{unit\ cell} = a^3 = 0.0147\ nm^3$

$\sqrt{3}a = r = 0.424$ nm

volume = $4/3\ \pi r^3 = 4/3\ \pi\ (0.424)^3 = 0.319\ nm^3$

Packing factor = 0.319/0.0147 = 21.7

1.12 The basic unit (or mer) of polytetrafluoroethylene (PTFE) or teflon is C_2F_4. If the mass of the PTFE molecule is 45,000 amu, what is the degree of polymerization ?

Basic unit $C_2F_4 = 2(12.01) + 4\,(19) = 100.02$ g

Molecular weight = n x molecule weight per mer (basic unit)

Degree of polymerization n = molecular weight /molecular weight per mer

$$n = 45000/100.02 \text{ g} \cong 450$$

1.13 Using the representation of the orthorhombic unit cell of polyethylene (see Figure Ex.1.13), calculate the theoretical density. How does this value compare with the density values of polyethylene obtained in practice?

There are 2 carbon atoms on each face, each of which is ½ inside the volume. Fore every C atom there are two H atoms. The unit cell volume thus has 4 C atoms to 8 H atoms.

$$\text{Volume} = (0.254 \text{ x } 10^{-7})(2.741 \text{ x } 10^{-2})(0.452 \text{ x } 10^{-7}) \text{ cm}^3$$
$$= 8.5073 \text{ x } 10^{-23} \text{ cm}^3$$

C→ 12 g/mol
H→ 1 g/mol

Thus, the density of polyethylene is

$$\rho = (12g/mol)(4atoms) + (1g/mol)(8atoms) \div (8.5073x10^{-23}cm^3)(6.02x10^{23}atoms/mol)$$
$$\rho = 1.093g/cm^3$$

In comparison, the density of high density polyethylene (HDPE), that is 95% crystalline, is about 0.95 – 0.96 g/cm^3

1.14 A pitch blend sample has five different molecular species with molecular masses of $0.5 \text{ x}10^{6}$, $0.5 \text{ x}10^{7}$, and $6 \text{ x}10^{7}$. Compute the number-averaged molecular weight and weight –averaged molecular weight of the sample.

Number-averaged molecular weight, $M_n = (\sum N_i M_i)/(\sum M_i)$

$M_n = (0.5\text{x}10^6 + 1 \text{ x } 10^7 + 4 \text{ x } 10^7 + 6 \text{ x } 10^7)/4$

$M_n = 27.625 \text{ x } 10^6$

Weight-averaged molecular weight, $M_w = (\sum N_i M_i^2)/(\sum N_i M_i)$

$M_w = (0.5\text{x}10^6)^2 + (1\text{x}10^7)^2 + (4\text{x}10^7)^2 +(6\text{x}10^7)^2 / \ 0.5\text{x}10^6 +1\text{x}10^7+6\text{x}10^7$

$M_w =47.966\text{x}10^6$

1.19 For a cubic system, calculate the angle between

(a) [100] and [111]

(b) [111] and [112]

(c) [112] and [221]

(a) [100] and [111]

$$v_1 = 1i + 0j + 0k$$
$$v_2 = 1i + 1j + 1k$$
$$\cos\alpha = \frac{1(1) + 0(1) + 0(1)}{\sqrt{1^2 + 0^2 + 0^2}\ \sqrt{1^2 + 1^2 + 1^2}} = \frac{1}{\sqrt{3}}$$
$$\alpha = 54.74^o$$

(b) [111] and [112]

$v_1 = 1i + 1j + 1k$
$v_2 = 1i + 1j - 2k$

$$\cos\alpha = \frac{1(1)+1(1)+1(-2)}{\sqrt{1^2+1^2+1^2}\sqrt{1^2+1^2+(-2)^2}} = 0$$

$\alpha = 90^o$

(c) [112] and [221]

$v_1 = 1i + 1j - 2k$
$v_2 = 2i + 2j + 1k$

$$\cos\alpha = \frac{1(2)+1(2)+(-2)(1)}{\sqrt{1^2+1^2+(-2)^2}\sqrt{2^2+2^2+1^2}} = \frac{2}{3\sqrt{6}}$$

$\alpha = 74.2^o$

1.20 Recalculate the bicycle stiffness ratio for a titanium frame. (See Examples 1.1 and 1.2) Find the stiffness and weight of the bicycle if the radius of the tube is 25 mm. Use the following information:

Alloy: Ti ---6% Al ---4% V,
σ_y = 1, 150MPa,
Density = 4.5 g/cm^3,
E = 106 GPa,
G = 40 GPa.

Solution:

$\rho = 4.5g/cm^3$
$\sigma y = 1150MPa$
$E = 106GPa$
$G = 40GPa$

	Steel	Ti
$\rho/\sigma y$	5.77 $\frac{kg}{MPa*m^3}$	3.9 $\frac{kg}{MPa*m^3}$
ρ/E	37.14 $\frac{kg}{GPa*m^3}$	42.5 $\frac{kg}{GPa*m^3}$

r_{Ti}= 2*r_{st}= 25mm

Find mass per length ratio:

$$\frac{m}{L} = \frac{2M\rho'}{r^2}(\frac{\rho}{E})$$

$$\frac{(\frac{m}{L})_{st}}{(\frac{m}{L})_{Ti}} = \frac{\frac{2M\rho_{st}'}{r_{st}^2}(\frac{\rho}{E})\Big|_{st}}{\frac{2M\rho_{Ti}'}{r_{Ti}^2}(\frac{\rho}{E})\Big|_{Ti}}$$

$$\frac{w_{st}}{w_{Ti}} = \frac{(\frac{m}{L})_{st}}{(\frac{m}{L})_{Ti}} = \frac{\frac{2M}{r_{st}}(\frac{\rho}{\sigma y})\Big|_{st}}{\frac{2M}{2r_{st}}(\frac{\rho}{\sigma y})\Big|_{Ti}} = \frac{2*5.77}{3.9} = 2.96$$

$$w_{Ti} = \frac{w_{st}}{2.96} = \frac{4kg}{2.96} = 1.35kg$$

$$\frac{\frac{2M}{r_{st}}(\frac{\rho}{\sigma y})\Big|_{st}}{\frac{2M}{4r_{st}}(\frac{\rho}{\sigma y})\Big|_{Ti}} = \frac{\frac{2M\rho_{st}'}{r_{st}^2}(\frac{\rho}{E})\Big|_{st}}{\frac{2M\rho_{Ti}'}{4r_{st}^2}(\frac{\rho}{E})\Big|_{Ti}}$$

$$2*2.96 = \frac{2\rho_{st}'}{\rho_{Ti}'}*\frac{37.14}{42.5}$$

$$\frac{\rho_{st}'}{\rho_{Ti}'} = 1.69 => \rho_{Ti}' = 0.59\rho_{st}'$$

1.21 Calculate the packing factor for NaCl, given that r_{Na} = 0.186 nm and r_{cl} = 0.107 nm.

$r_{Na} = .186nm \qquad r_{Cl} = .107nm$

<u>NaCl is FCC</u>

$$\begin{aligned} a_0 &= 2r_{Cl} + 2r_{Na} \\ &= 2(.186 + .107) \\ &= .586nm \end{aligned}$$

$$PF = \frac{(4)\frac{4}{3}\pi r_{Cl}{}^{3} + (4)\frac{4}{3}\pi r_{Na}{}^{2}}{a_0{}^{3}}$$

$$PF = \frac{\frac{16}{3}\pi\left((.186\times10^{-9})^3 + (.107\times10^{-9})^3\right)}{(.586\times10^{-9})^3} = .6377$$

1.22 **De**termine the density of BCC iron structure if the iron atom has a radius of 0.124 nm.

Iron radius = 0.124 nm

$$4r = a_0\sqrt{3}$$

$$\frac{4\sqrt{3}}{3}r = a_0$$

To calculate the # of atoms in the cell: $\left(8\times\frac{1}{8}\right) + (1\times1) = 2$

Atomic mass of Fe = 55.85 $\Rightarrow$ see Appendix, p. 846

$$\rho = \frac{2(55.85)}{\left(\frac{4\sqrt{3}}{3}r\right)^3(6.022\times10^{23})} = \frac{2(55.85)}{\left(\frac{4\sqrt{3}}{3}(.124\times10^{-9})\right)(6.02\times10^{23})}$$

$$\rho_{BCC} = .7901208\frac{g}{m^3} = \boxed{7.901\frac{g}{cm^3}}$$

1.24 Calculate the stress generated in a turbine blade if its cross-sectional area is 0.002 m^2 and the mass of each blade is 0.5 kg. Assume that the rotational velocity ω = 15,000 rpm and the turbine disk radius is 1 m.

The centripetal acceleration at the tip of each turbine blade is:

$$a_c = \omega^2 R = (15000 * 1/60 * 2\pi)^2 * 1 = 2.47 * 10^6 m/s^2$$

The stress generated is:

$$\sigma = \frac{F}{A} = \frac{ma_c}{A} = \frac{0.5 * 2.47 * 10^6}{0.002} = 6.7MPa$$

1.25 Suppose that the turbine blade from the last problem is part of a jet turbine. The material of the jet turbine is a nickel-based superalloy with the yield strength, σ_y = 1.5 GPa; it decreases with temperature as

$\sigma = \sigma_0[(1 - (T - T_0))/(T_m - T_0)],$

where T_0 = 293 K is the room temperature and T_m = 1,550 K is the melting temperature. Find the temperature at which the turbine will flow plastically under the influence of centripetal forces.

We have

$$\sigma_o = 1.5\ GPa$$
$$T_o = 293 K$$
$$T_m = 1550 K$$
$$\sigma = 6.7\ MPa\ (\textit{from the previous problem})$$

The temperature at which the turbine flows plastically under the influence of the centripetal force:

$$T = (1 - \frac{\sigma}{\sigma_0})(T_m - T_0) + T_0 = (1 - \frac{6.7 * 10^6}{1.5 * 10^4})(1550 - 293) + 293 = 1033K$$

1.27 A jet turbine blade, made of MARM 200 (a nickel-based superalloy) rotates at 10,000 rpm. The radius of the disk is 50 mm. The cross-sectional area is 20 cm^2 and the length of the blade is equal to 12 cm. The density of MARM200 is 8.5 g/cm^3.

(a) What is the stress acting on the turbine blade in MPa?
(b) If the room temperature strength of MARM 200 is equal to 800 MPa, what is the maximum operational temperature in Kelvin?

The yield stress varies with temperature as:

$$\sigma = \sigma_0 \left(1 - \left[\frac{(T - T_0)}{(T_m - T_0)}\right]^m\right)$$

where T_m is the melting temperature (T_m = 1,700 K) and T_0 is the room temperature; m = 0.5.

a)

$$\begin{aligned}
&Given:\\
&velocity = \omega = 10{,}000\,rpm\\
&r = 50mm = 0.05m\\
&A_\circ = 20cm^2 = 0.002m^2\\
&\ell = 12cm = 0.12m\\
&\rho = 8.5\,g/cm^3 = 8.5\times10^6\,g/m^3\\
&Find:\\
&\sigma = \frac{F}{A} = \frac{ma_c}{A_\circ}\\
&a_c = \omega^2 r = \left[10{,}000\,rpm * \frac{1m}{60s} * 2\pi\right] * 0.05m = 5.48\times10^4\,m/s^2\\
&m = \rho A_\circ \ell = 8.5\times10^6\,g/m^3 * 0.002m^2 * 0.12m = 2040g = 2.04kg\\
&So:\\
&\sigma = \frac{2.04kg * 5.48\times10^4\,m/s^2}{0.002m^2} = 5.59\times10^7\,g\cdot m/s^2 = 55.8\,MPa
\end{aligned}$$

$$\sigma = \sigma_{\circ}\left[1-\left(\frac{(T-T_{\circ})}{(T_m-T_{\circ})}\right)^m\right]$$

$$T_m = 1700K$$

$$m = 0.5$$

$$\sigma_{RT} = 800\,MPa$$

$$At\ room\ temperature\ (\approx 294K):$$

$$800\ MPa = \sigma_{\circ}\left[1-\left(\frac{(T_{\circ}-T_{\circ})}{(T_m-T_{\circ})}\right)^m\right]$$

$$Therefore:$$

$$\sigma_{\circ} = 800\,MPa$$

$$The\ \max\ temperature\ is:$$

$$55.8MPa = 800MPa\left[1-\left(\frac{(T-294K)}{(1700K-294K)}\right)^{0.5}\right]$$

$$0.06975 = 1-\left(\frac{(T-294K)}{(1406K)}\right)^{0.5}$$

$$0.93025 = \left(\frac{(T-294K)}{(1406K)}\right)^{0.5}$$

$$0.86536 = \frac{T-294K}{1406K}$$

$$1216K = T-294K$$

$$T_{\max} = 1510K$$

1.28 Generate a three-dimensional unit cell for the intermetallic compound $AuCu_3$ that has a cubic structure. The Au atoms are at the cube corners and the Cu atoms at the center of the faces. Given:

r_{Cu} = 0.128 nm *A.N.* Cu = 63.55 amu

r_{Au} = 0.144 nm *A.N.* Au = 196.97 amu

(a) Find the lattice parameter in nanometers.

(b) What is the atomic mass of the unit cell in grams?

(c) What is the density of the compound in g/cm3?

(a) The lattice parameter in nanometers is:

$$2(r_{Cu} + r_{Ag}) = \sqrt{2}a_0$$

$$a_0 = \sqrt{2}(r_{Cu} + r_{Ag}) = \sqrt{2}(0.128 + 0.144) = 0.385nm$$

(b) The atomic mass of the unit cell in grams is:

$$Ag + 3Cu = m = \frac{63.55 * 3 + 196.97}{6.02 * 10^{23}} = 6.44 * 10^{-22} g$$

(c) The density if the compound in g/cm^3 is:

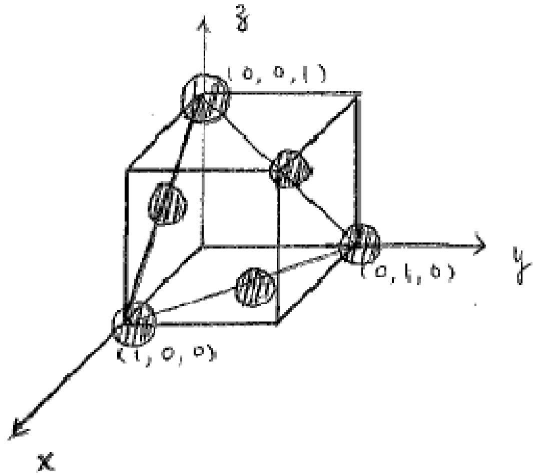
$$\rho = \frac{m}{v} = 6.44 * 10^{-22} / (0.385 * 10^{-7})^3 = 11.28 g / cm^3$$

1.30. Show how the atoms pack in the following planes by drawing circles (atoms) in the appropriate spots:

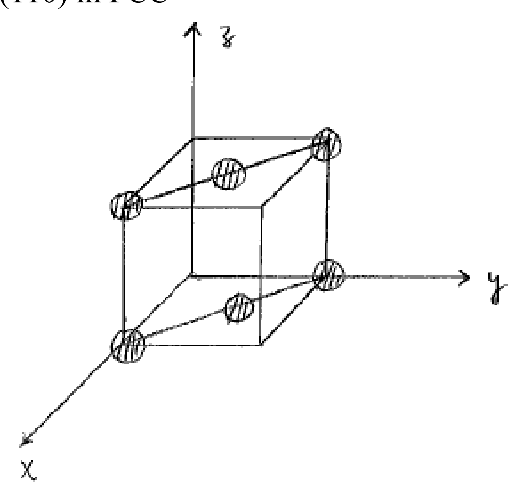
(a) (111) in FCC,
(b) (110) in FCC,
(c) (111)in BCC,
(d) (110)in BCC.

Solution:

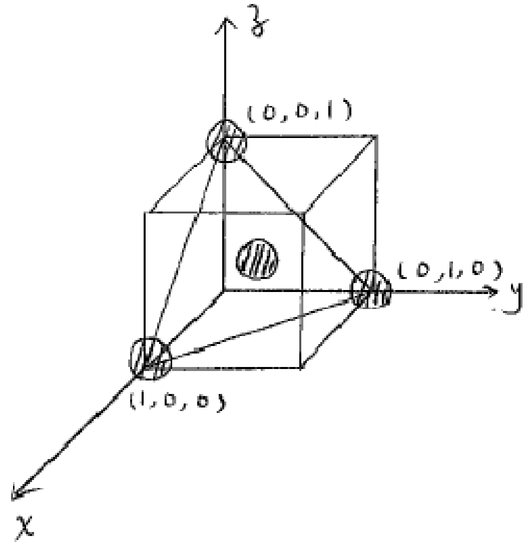
(a) (111) in FCC



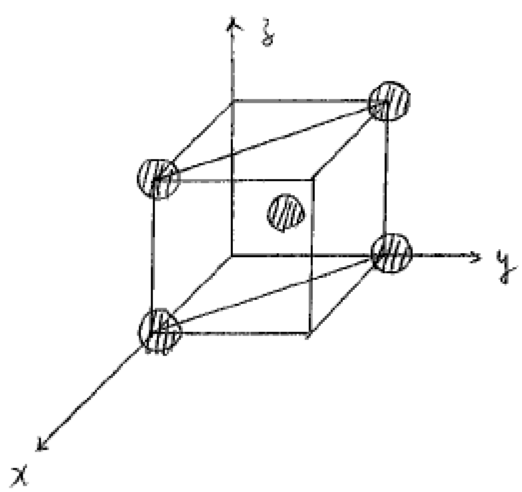
(b) (110) in FCC



(c) (111) in BCC



(d) (110) in BCC



1.35 Calculate the APF (atomic packing factor) for BCC and FCC unit cells, assuming the atoms are represented as hard spheres. Do the same for the diamond cubic structure.

Packing factor = (# of atoms per cell) (volume of atom) ÷ (total volume)

Assuming the atoms to be spheres, we can write

Volume of atom = $\frac{4}{3}\pi r^3$

Total volume of the unit cell cube $= a_0{}^3$

Structure	# of atoms per cell	a_0
BCC	$8\cdot\left(\frac{1}{8}\right)+1(1)=2$	$\frac{4r}{\sqrt{3}}$
FCC	$8\cdot\left(\frac{1}{8}\right)+6\left(\frac{1}{2}\right)=4$	$\frac{4r}{\sqrt{2}}$
Diamond Cubic	$8\cdot\left(\frac{1}{8}\right)+6\left(\frac{1}{2}\right)+4=8$	$\frac{8r}{\sqrt{3}}$

Packing factors

$$\text{BCC} = \frac{(2)\left(\frac{4}{3}\pi r^3\right)}{\left(\frac{4r}{\sqrt{3}}\right)^3} = \frac{2\left(\frac{4}{3}\right)\pi r^3}{\left(\frac{4}{\sqrt{\ }}\right)^3 r^3} = \frac{\frac{8}{3}\pi}{\frac{648}{3\sqrt{3}}} \approx .68$$

$$\text{FCC} = \frac{(4)\left(\frac{4}{3}\pi r^3\right)}{\left(\frac{4}{\sqrt{2}}r\right)^3} = \frac{4\cdot\left(\frac{4}{3}\right)\pi r^3}{\frac{4^3}{\left(\sqrt{2}\right)^3}r^3} = \frac{\frac{\pi}{3}}{\frac{2}{\sqrt{2}}} \approx .74$$

$$\text{Diamond Cubic} = \frac{(8)\left(\frac{4}{3}\pi r^3\right)}{\left(\frac{8r}{\sqrt{3}}\right)^3} \approx .34$$

1.37. A block copolymer has macromolecules of each polymer attached to the other as can be seen in Figure 1.22(c). The total molecular weight is 100,000 g/mol. If 140 g of A and 60 g of B were added, determine the degree of polymerization for each polymer. A: 56 g/mol; B: 70 g/mol.

Total MW=100,000g/mol
140g of A
60g of B
A:B=7:3
Determine degree of polymerization for each polymer:
A:56g/mol
B:70g/mol
MWA=70,000g/mol
MWB=30,000g/mol

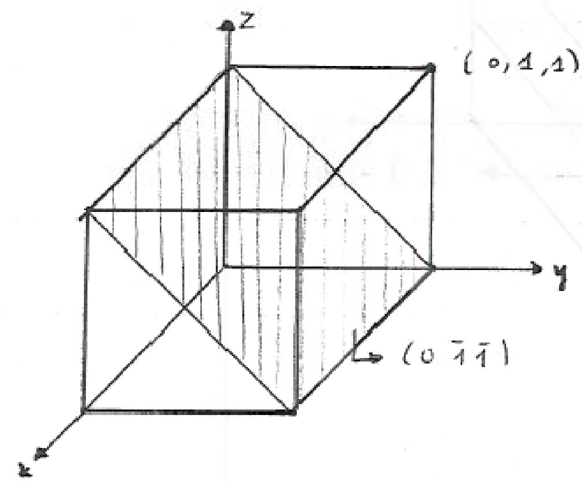
$$DP_A = \frac{MW_A}{7 * MWofA} = \frac{70,000g/mol}{7*56g/mol} = 179$$

$$DP_B = \frac{MW_B}{3 * MWofB} = \frac{30,000g/mol}{3*70g/mol} = 143$$

1.38. Sketch the following planes within the unit cell. Draw one cell for each solution. Show new origin and ALL necessary calculations.

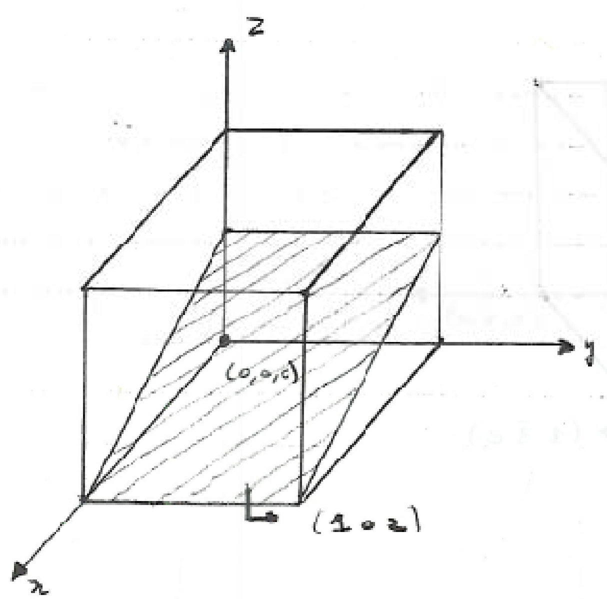
(a) $(0\bar{1}\bar{1})$,

⇒ intersections $\left(\infty, \frac{1}{-1}, \frac{1}{-1}\right)$, origin (0, 1, 1)



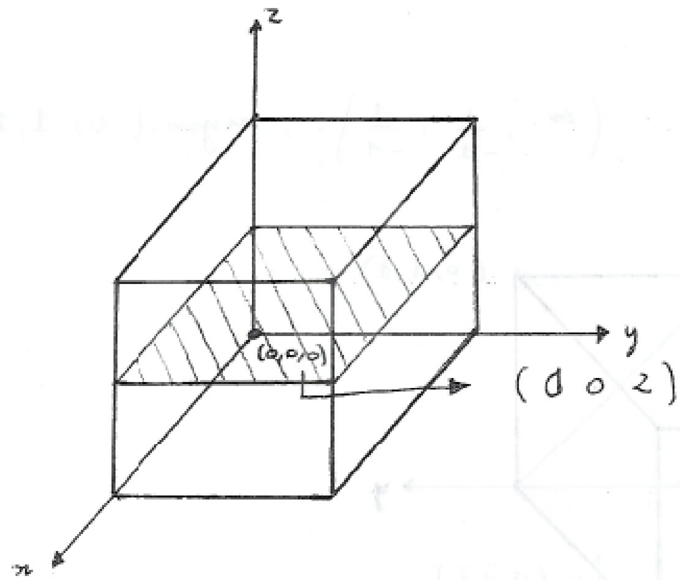
(b) (102),

⇒ intersections: $\left(\frac{1}{1}, \infty, \frac{1}{2}\right)$ origin (0,0,0)



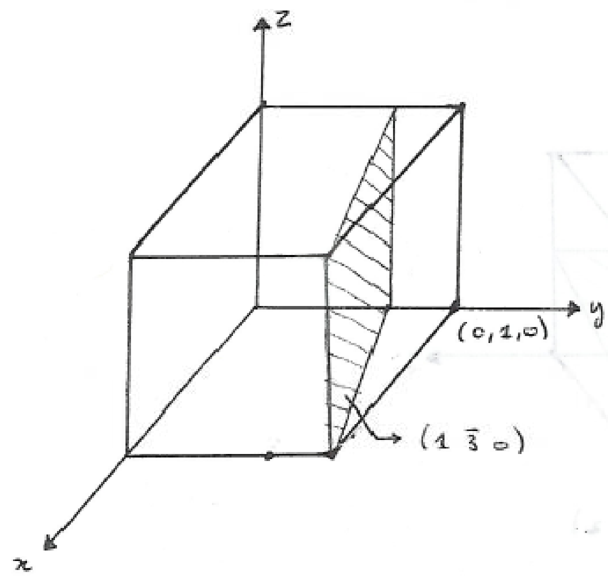
(c) (002),

⇒ intersections $(\infty, \infty, \frac{1}{2})$ origin $(0,0,0)$



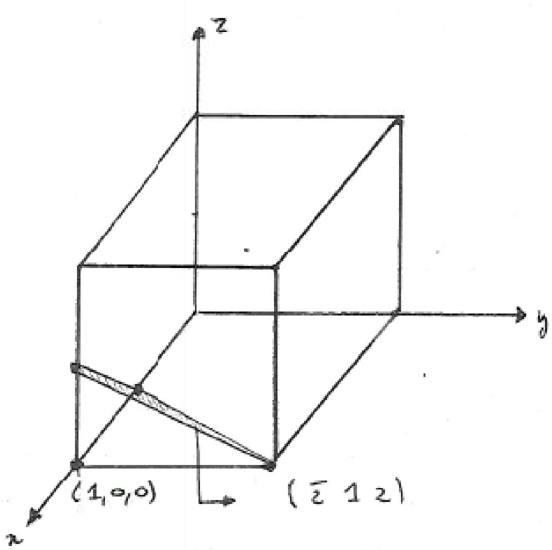
(d) $(1\bar{3}0)$,

⇒ intersections $(1, -\frac{1}{3}, \infty)$ origin $(0,1,0)$



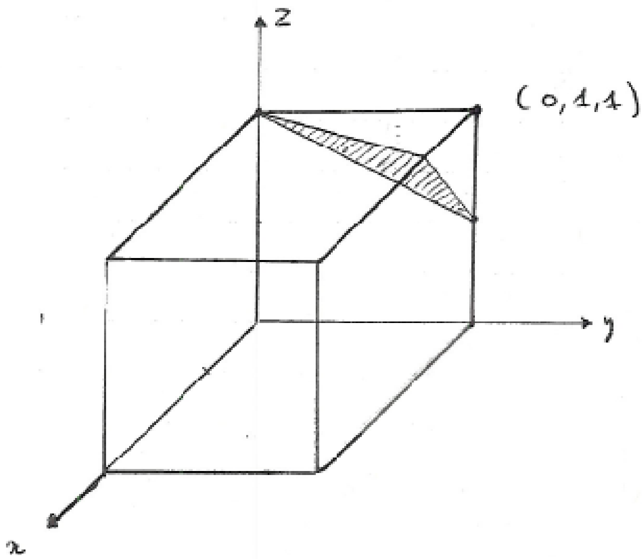
(e) $(\bar{2}12)$,

⇒ intersections $(-\frac{1}{2}, 1, \frac{1}{2})$ origen $(1,0,0)$



(f) $(3\overline{1}\overline{2})$

⇒ intersections $\left(\frac{1}{3}, -\frac{1}{1}, -\frac{1}{2}\right)$ origin $(0,1,1)$



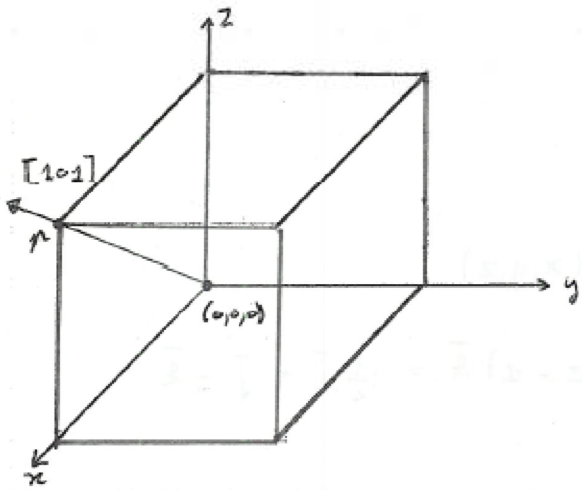
1.39. Sketch the following directions within the unit cell. Draw one cell for each solution. Show new origin and ALL necessary calculations.

a) [1 0 1] $\Rightarrow \bar{v} = \bar{i} + \bar{k}$

origin (0,0,0) point p(x, y, z)

$\Rightarrow \bar{v} = (x-0)\bar{i} + (y-0)\bar{j} + (z-0)\bar{k} = \bar{i} + \bar{k}$

$$\Rightarrow \begin{cases} x = 1 \\ y = 0 \\ z = 1 \end{cases}$$

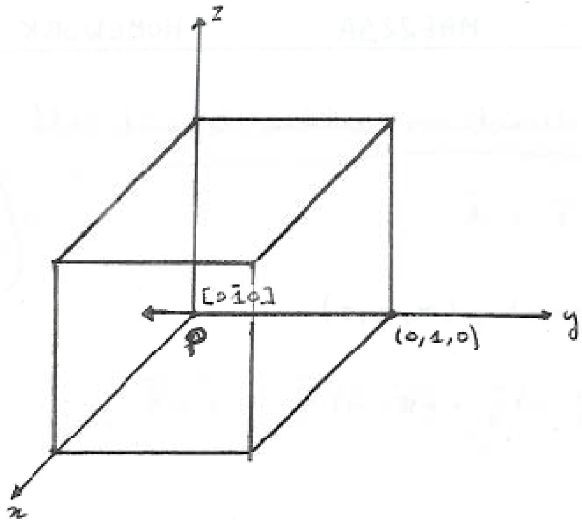


b) [0 $\bar{1}$ 0] $\Rightarrow \bar{v} = -\bar{j}$

origin (0,1,0) point p(x, y, z)

$\Rightarrow \bar{v} = (x-0)\bar{i} + (y-1)\bar{j} + (z-0)\bar{k} = -\bar{j}$

$$\Rightarrow \begin{cases} x = 0 \\ y = 0 \\ z = 0 \end{cases}$$



a) [1 2 $\bar{2}$]

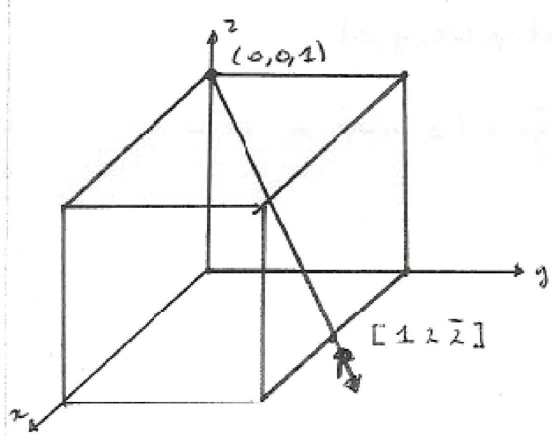
$2\bar{v} = \bar{i} + 2\bar{j} - 2\bar{k}$

$\bar{v} = \frac{1}{2}\bar{i} + \bar{j} - \bar{k}$

origin (0,0,1) point p(x,y,z)

$\Rightarrow \bar{v} = (x-0)\bar{i} + (y-0)\bar{j} + (z-1)\bar{k} = \frac{1}{2}\bar{i} + \bar{j} - \bar{k}$

$\Rightarrow \begin{cases} x = \frac{1}{2} \\ y = 1 \\ z = 0 \end{cases}$



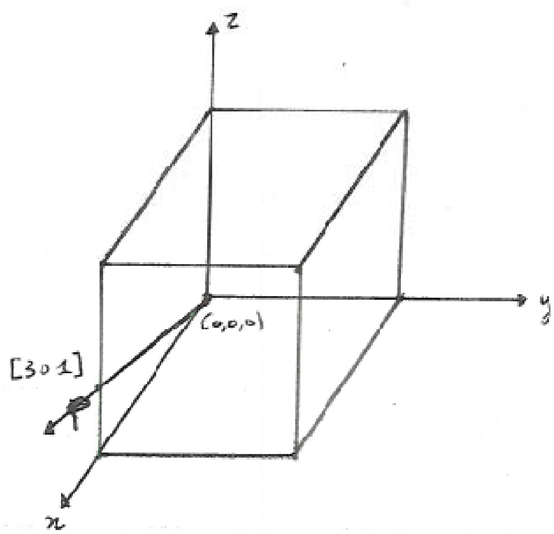
b) [3 0 1]

$3\bar{v} = 3\bar{i} + \bar{k}$
$\bar{v} = \bar{i} + \frac{1}{3}\bar{k}$

origin (0,0,0) point p(x,y,z)

$\Rightarrow \bar{v} = (x-0)\bar{i} + (y-0)\bar{j} + (z-0)\bar{k} = \bar{i} + \frac{1}{3}\bar{k}$

$\Rightarrow \begin{cases} x = 1 \\ y = 0 \\ z = \frac{1}{3} \end{cases}$



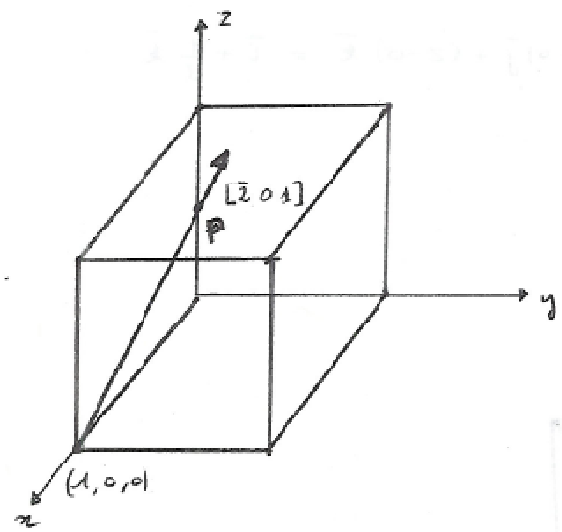
c) [$\bar{2}$ 0 1]

$2\bar{v} = -2\bar{i} + \bar{k}$
$\bar{v} = -\bar{i} + \frac{1}{2}\bar{k}$

origin (1, 0, 0) point p(x,y,z)

$\Rightarrow \bar{v} = (x-1)\,\bar{i} + (y-0)\,\bar{j} + (z-0)\,\bar{k} = -\bar{i} + \frac{1}{2}\,\bar{k}$

$$\Rightarrow \begin{cases} x = 0 \\ y = 0 \\ z = \frac{1}{2} \end{cases}$$



d) [2 $\bar{1}$ 3]

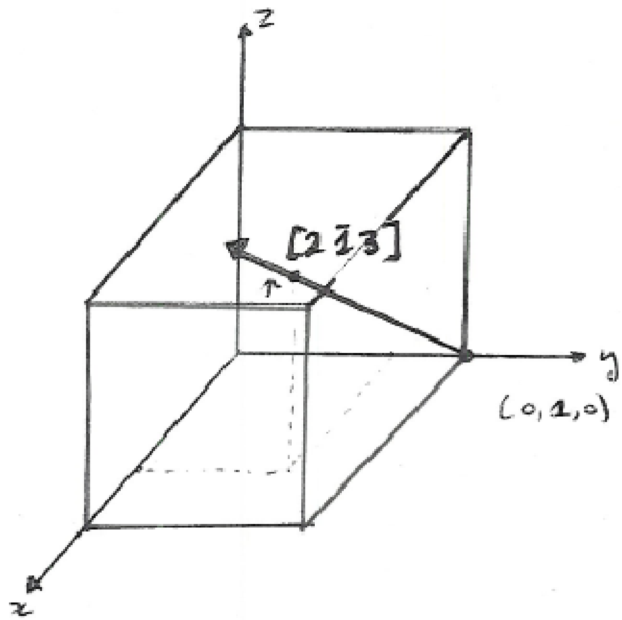
$3\,\bar{v} = 2\,\bar{i} - \bar{j} + 3\,\bar{k}$

$\bar{v} = \frac{2}{3}\,\bar{i} - \frac{1}{3}\,\bar{j} + \bar{k}$

origin (0, 1, 0) point p (x, y, z)

$\Rightarrow \bar{v} = (x-0)\,\bar{i} + (y-1)\,\bar{j} + (z-0)\,\bar{k} = \frac{2}{3}\,\bar{i} - \frac{1}{3}\,\bar{j} + \bar{k}$

$$\Rightarrow \begin{cases} x = \frac{2}{3} \\ y = \frac{2}{3} \\ z = 1 \end{cases}$$


z
[2 $\bar{1}$ 3]
y
(0,1,0)
x

1.40. Suppose we introduce one carbon atom for every 100 iron atoms in an interstitial position in BCC iron, giving a lattice parameter of 0.2867 nm. For the Fe–C alloy, find the density and the packing factor.

Given:

Atomic mass of C = 12,

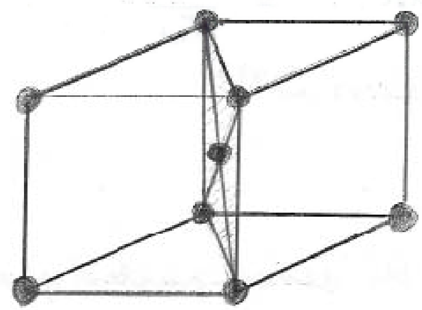
Atomic mass of Fe = 55.89,

a(Fe) = 0.2867 nm,

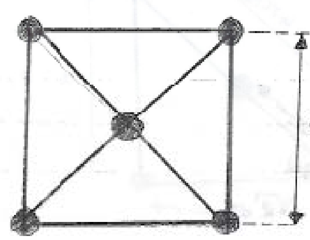
Avogadro's number, $N = 6.02 \times 10^{23}$

<u>Solution</u>:

BCC iron :



densest packed plane :



- $\rho = \dfrac{m}{V}$ $\qquad V = (0{,}2867 \cdot 10^{-7})^3$

- m ?

There are 2 atoms Fe in one 'unit cell' BCC-Fe.

.

There is 1 C - atom for every 100 Fe - atoms

$\Rightarrow$ thus for 2 Fe - atoms, we will have $\frac{1}{50}$ C-atoms

$$m = \frac{A.M.}{N_A} = \frac{\left[(55{,}85 \times 2) + (12 \times \frac{1}{50})\right]}{6{,}02 \cdot 10^{23}}$$

- $$\rho = \frac{m}{V} = \frac{\left[(55{,}85 \times 2) + (12 \times \frac{1}{50})\right]}{(6{,}02 \cdot 10^{23}) \times (0{,}2867 \cdot 10^{-7})^3} = 7{,}896 \ g/cm^3$$

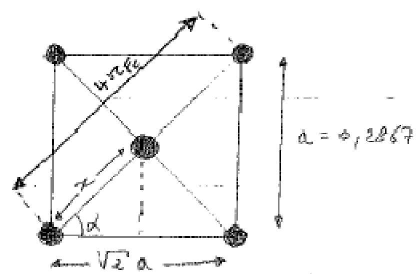
$$\boxed{\rho = 7{,}896 \ g/cm^3}$$

- Packing factor? $= \frac{V_{Fe}}{V_{tot}}$

$V_{tot} = V = (0{,}2867 \cdot 10^{-7})^3$

V_{Fe} ?

If we look at the densest packed plane :



$$tg\,\alpha = \frac{a}{2} \cdot \frac{2}{\sqrt{2}\,a} = \frac{1}{\sqrt{2}} \Rightarrow \alpha = 35{,}2643°$$

$$\sin\alpha = \frac{a}{2} \cdot \frac{1}{x} \Rightarrow x = \frac{a}{2 \cdot \sin\alpha} = \frac{a}{2 \cdot \frac{\sqrt{3}}{3}} = \frac{3}{2}\,\frac{a}{\sqrt{3}} = \frac{\sqrt{3}}{2}\,a$$

$$\Rightarrow 4 r_{Fe} = 2x = \sqrt{3}\,a$$

$$\Rightarrow r_{Fe} = \frac{\sqrt{3}\,a}{4} = \frac{\sqrt{3} \cdot 0{,}2867 \cdot 10^{-7}}{4}$$

2 atoms of Fe in 1 Unit Cell BCC-Fe

$$\Rightarrow V_{Fe} = 2 \times \Big[\underbrace{\tfrac{4}{3} \pi r_{Fe}^3}_{\text{Volume of 1 iron atom}} \Big]$$

$$\Rightarrow V_{Fe} = 2 \times \left[\frac{4}{3} \pi \left(\frac{\sqrt{3} . 0,2867.10^{-7}}{4} \right)^3 \right] = 1,60289 . 10^{-23}$$

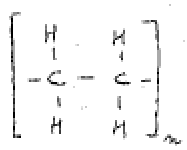
$$\Rightarrow \text{Packing factor} = \frac{V_{Fe}}{V_{tot}} = \frac{1,60289 . 10^{-23}}{(0,2867 . 10^{-7})^3} = 0,6802$$

$\Rightarrow$ **Packing factor = 0,6802**

1.42. Determine the maximum length of a polymer chain made with 1,500 molecules of ethylene, knowing that the carbon bond length is 0.13 nm.

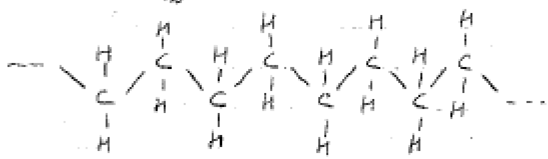
Solutions:

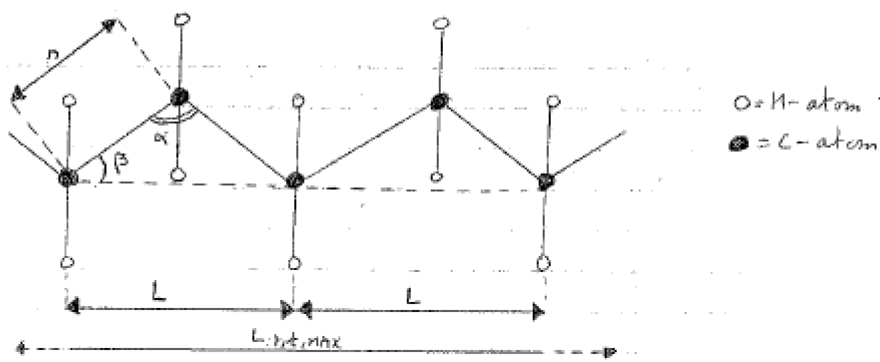
ethylene :



and $n = 1500$

polyethylene :





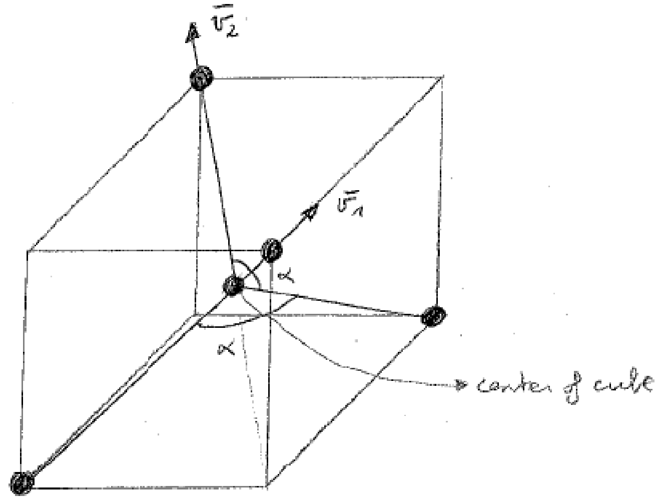
Polyethylene is a linear polymer. The chain has the maximum length if there are no curves!

$L_{tot,MAX} = n \cdot L = 1500 \cdot L$

$L = 2 \cdot s \cdot \cos\beta$ and $s = 2 \cdot r_c = 2 \cdot 0,013 \cdot 10^{-9}$

What is β? To find β, we have to find α first!

To find α, we place a C-atom in the center of a unit box, bonded with 4 other atoms on the edges of the box.



We now define 2 vectors: $\bar{v}_1$ and $\bar{v}_2$, which allow us to solve the problem vectorwise.

$$\bar{v}_1 = \frac{1}{2}\bar{i} + \frac{1}{2}\bar{j} + \frac{1}{2}\bar{k}$$

$$\bar{v}_2 = -\frac{1}{2}\bar{i} - \frac{1}{2}\bar{j} + \frac{1}{2}\bar{k}$$

$$\Rightarrow \cos \measuredangle(\bar{v}_1, \bar{v}_2) = \frac{(\bar{v}_1, \bar{v}_2)}{\|\bar{v}_1\| \cdot \|\bar{v}_2\|}$$

$$\Rightarrow \cos \measuredangle(\bar{v}_1, \bar{v}_2) = \frac{\left(\frac{1}{2}\right)\cdot\left(-\frac{1}{2}\right) + \left(\frac{1}{2}\right)\left(-\frac{1}{2}\right) + \left(\frac{1}{2}\right)\cdot\left(\frac{1}{2}\right)}{\sqrt{\left(\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2} \cdot \sqrt{\left(-\frac{1}{2}\right)^2 + \left(-\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2}}$$

$$= \frac{-\frac{1}{4} - \frac{1}{4} + \frac{1}{4}}{\sqrt{\frac{3}{4}} \cdot \sqrt{\frac{3}{4}}} = \frac{-1/4}{3/4} = -\frac{1}{3}$$

$$\Rightarrow \cos \alpha = \cos(\bar{v}_1, \bar{v}_2) = 109,47^\circ$$

$$2\beta = 180 - \alpha$$

$$\beta = \frac{180 - 109.47}{2} = 35.265°$$

$$L_{Total,\,Max} = 1500 * 2 * 2 * 0.013 * 10^{-9} * \cos(35.265°) = 6.33 * 10^{-8}\, m$$