Fundamentals of Materials Science Homework 9

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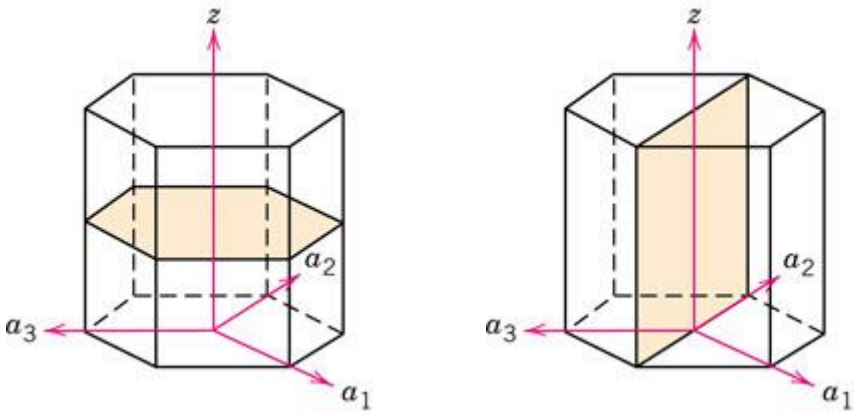
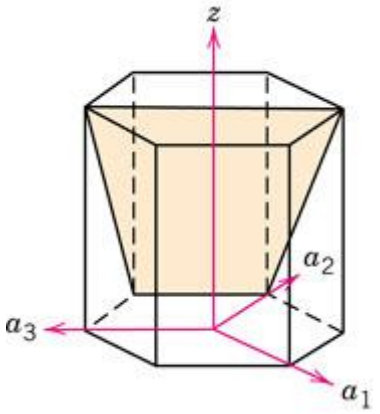
Homework Problems:

1. Determine the *Miller-Bravais* indices for the planes shown in the following unit cells:

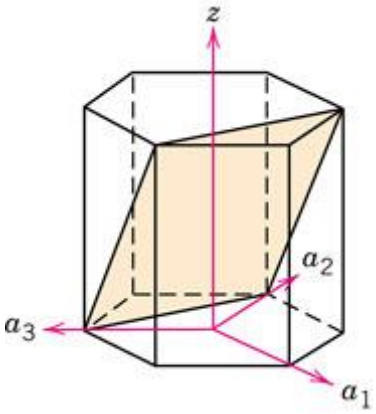


(a)

(b)



(c)



(d)

Solution:

(a) $\because a_1 = \infty a; a_2 = \infty a; z = \frac{1}{2}c$

$\therefore h = 0; k = 0; l = 2; i = -(h+k) = 0$

$\therefore (0001)$

(b) $\because a_1 = a; a_2 = \infty a; z = \infty c$

$\therefore h=1; k=0; l=0; i=-(h+k)=-1$

$\therefore (10\bar{1}0)$

(c) $\because a_1=-a; a_2=a; z=c$

$\therefore h=-1; k=1; l=1; i=-(h+k)=0$

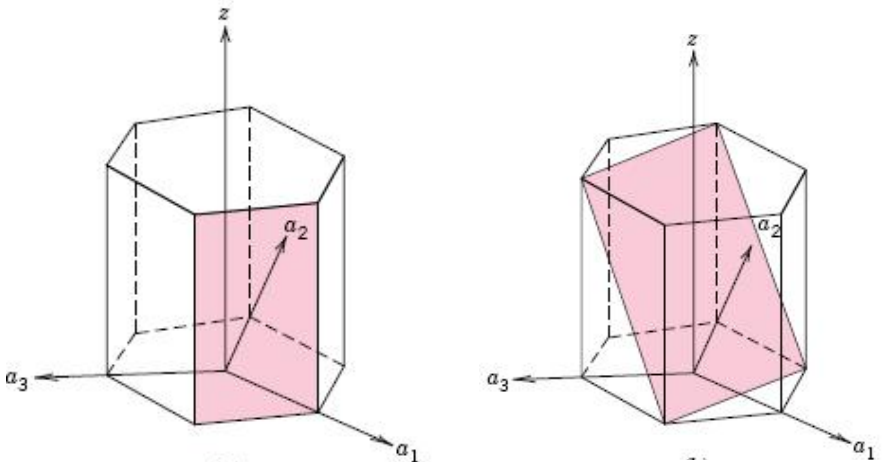
$\therefore (\bar{1}101)$

(d) $\because a_1=-\frac{1}{2}a; a_2=a; z=\frac{1}{2}c$

$\therefore h=-2; k=1; l=2; i=-(h+k)=1$

$\therefore (\bar{2}112)$

2. Determine the *Miller-Bravais* indices for the planes shown in the following unit cells:



(a) **(b)**

Solution:

(a) $\because a_1=a; a_2=-a; z=\infty c$

$\therefore h=1; k=-1; l=0; i=-(h+k)=0$

$\therefore (1\bar{1}00)$

(b) $\because a_1=\frac{1}{2}a; a_2=-a; z=\frac{1}{2}c$

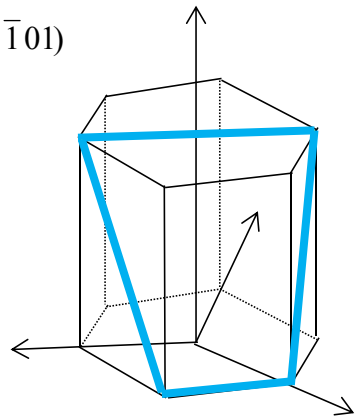
$\therefore h=2; k=-1; l=2; i=-(h+k)=-1$

$\therefore (2\bar{1}\bar{1}2)$

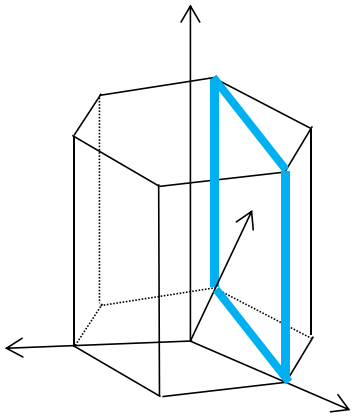
3. Sketch the $(1\bar{1}01)$ and $(11\bar{2}0)$ planes in a hexagonal unit cell.

Solution:

$(1\bar{1}01)$



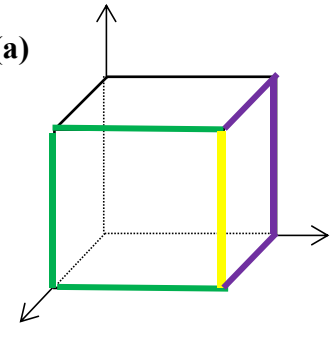
$(11\bar{2}0)$



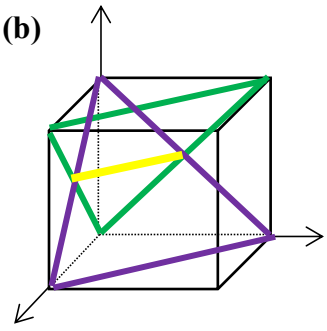
4. Cite the indices of the direction that results from the intersection of each of the following pairs of planes within a cubic crystal: (a) the (100) and (010) planes, (b) the (111) and $(11\bar{1})$ planes, (c) the $(10\bar{1})$ and (001) planes.

Solution:

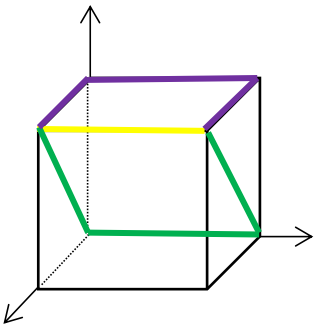
(a)



(b)



(c)



5. For the HCP crystal structure, show that the ideal c/a ratio is 1.633. Calculate the atomic packing fraction for the hexagonal close-packed crystal structure for which $c = a\sqrt{8/3}$. Remember that the base of the unit cell is a parallelogram.

Solution:

$$APF_{HCP}=\frac{nV_1}{V}=\frac{6\times\frac{4}{3}\pi r^3}{\frac{3\sqrt{3}}{2}a^2\sqrt{\frac{8}{3}}a}=\frac{6\times\frac{4}{3}\pi\left(\frac{a}{2}\right)^3}{3\sqrt{2}a^3}=0.74$$

6. Zirconium has an HCP crystal structure and a density of 6.51 g/cm³.
(a) What is the volume of its unit cell in cubic meters?
(b) If the *c*/*a* ratio is 1.593, compute the values of *c* and *a*.

Solution:

(a) Atomic weight of Zr : 91.22amu
Density of Zr : 6.51g/cm³
∵ Zirconium has an HCP crystal structure; ∴ n=6

$$V_{Zr}=\frac{nA}{\rho N_A}=\frac{6\times 91.22amu}{6.51g/cm^3\times 6.02\times 10^{23}atoms/mol}=1.4\times 10^{-28}m^3$$

(b) $V_{HCP}=3\times a\times\frac{\sqrt{3}a}{2}\times c$

$$\because \frac{c}{a}=1.593\therefore V_{HCP}=3\times a\times\frac{\sqrt{3}a}{2}\times 1.593a=1.4\times 10^{-28}m^3$$

$$\therefore a=0.323nm; c=1.593a=0.515nm$$

7. Rhodium has an atomic radi s of 0.1345 nm (1.345Å) and a density of 12.41 u g/cm³. Determine whether it has an FCC or BCC crystal structure.

Solution:

Atomic weight of Rh : 102.91amu
Density of Rh : 12.41g/cm³
atomic radius : 0.1345nm

(1) FCC: $\rho=\frac{nA}{V_{Rh}N_A}=\frac{4\times 102.91amu}{\left(2\sqrt{2}\times 0.1345nm\right)^3\times 6.02\times 10^{23}atoms/mol}=12.41g/cm^3$

(2) BCC: $\rho=\frac{nA}{V_{Rh}N_A}=\frac{2\times 102.91amu}{\left(\frac{4}{\sqrt{3}}\times 0.1345nm\right)^3\times 6.02\times 10^{23}atoms/mol}=11.40g/cm^3$

So it has FCC crystal structure.

8. Beryllium (Be) has an HCP unit cell for which the ratio of the lattice parameters c/a is 1.568. If the radius of the Be atom is 0.1143 nm, (a) determine the unit cell volume, and (b) calculate the theoretical density of Be and compare it with the literature value.

Solution:

$$\text{(a) } V_{HCP} = \frac{3\sqrt{3}a}{2}a^2 \times c = \frac{3\sqrt{3}}{2} \times 1.568(2R)^3$$

$$= \frac{3\sqrt{3}}{2} \times 1.568 \times (2 \times 0.1143nm)^3 = 4.867 \times 10^{-23} cm^3$$

$$\text{(b) } \rho = \frac{nA}{V_{Be}N_A} = \frac{6 \times 9.012 g/mol}{4.867 \times 10^{-23} cm^3 \times 6.02 \times 10^{23} atoms/mol} = 1.845 g/cm^3$$

the theoretical density of Be is 1.845g/mol
the literature value is 1.85g/mol

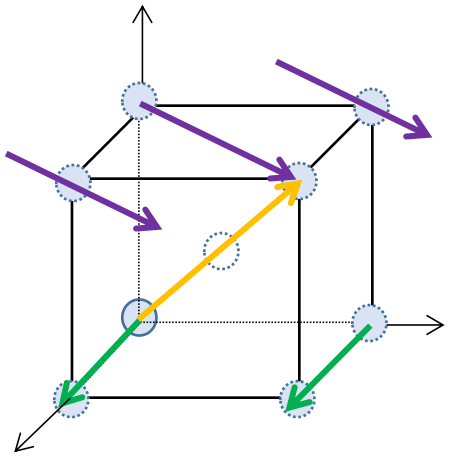
9. Calculate and compare the linear densities for the <100>, <110> and <111> directions in a BCC unit cell. Which direction is the most close-packed (dense)?

Solution:

<1 1 0> $LD_{110} = \frac{1}{\sqrt{2}a} = \frac{1}{\sqrt{2}\frac{4}{\sqrt{3}}R} = \frac{3}{4\sqrt{6}R}$

<1 0 0> $LD_{100} = \frac{1}{a} = \frac{1}{\frac{4}{\sqrt{3}}R} = \frac{\sqrt{3}}{4R}$

<1 1 1> $LD_{111} = \frac{2}{\sqrt{3}a} = \frac{2}{\sqrt{3}\frac{4}{\sqrt{3}}R} = \frac{1}{2R}$



$\because LD_{110} < LD_{100} < LD_{111}$ $\therefore$ <111>is the most close-packed (dense).

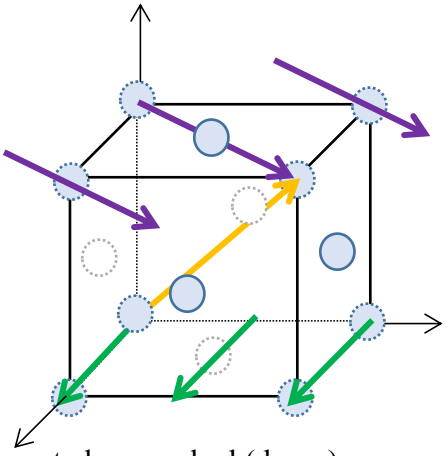
10. Calculate and compare the linear densities for the <100>, <110> and <111> directions in a FCC unit cell. Which direction is the most close-packed (dense)?

Solution:

<1 1 0> $LD_{110} = \frac{2}{\sqrt{2}a} = \frac{2}{4R} = \frac{1}{2R}$

<1 0 0> $LD_{100} = \frac{1}{a} = \frac{1}{2\sqrt{2}R}$

<1 1 1> $LD_{111} = \frac{1}{\sqrt{3}a} = \frac{1}{2\sqrt{6}R}$



$\because LD_{111} < LD_{100} < LD_{110}$ $\therefore$ <110>is the most close-packed (dense).

10. Suppose that FCC rhodium is produced as a 1-mm thick sheet, with the (111) plane parallel to the surface of the sheet. How many (111) interplanar spacings d_{III} thick is the sheet? See Appendices in your textbook for necessary data.

Solution:

Lattice parameter:0.38044nm

$$\because d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \therefore d_{111} = \frac{0.38044nm}{\sqrt{3}} = 0.22nm$$

$$n = \frac{1mm}{d_{111}} = \frac{10^6 nm}{0.22nm} = 4.55 \times 10^6$$

11. Determine the minimum radius of an atom that will just fit into (a) the tetrahedral interstitial site in FCC nickel; and (b) the octahedral interstitial site in BCC lithium.

Solution:

(a)$\because$Ni is tetrahedral in FCC $\therefore$Coordination number is 4

$\therefore r_c/r_a$ range:0.225~0.414

Lattice parameter of Ni is 0.35236nm

$$\therefore r_{Ni} = \frac{a}{2\sqrt{2}} = \frac{0.35236nm}{2\sqrt{2}} = 0.12360nm$$

$$\therefore \frac{r_{\min}}{r_{Ni}} = 0.225; r_{\min} = 0.225 \times 0.12360nm = 0.02781nm$$

(b)$\because$Li is octahedral in BCC $\therefore$Coordination number is 8

$\therefore r_c/r_a$ range:0.414~0.732

Lattice parameter of Ni is 0.35089nm

$$\therefore r_{Li} = \frac{a}{\frac{4}{\sqrt{3}}} = \frac{0.35089nm}{\frac{4}{\sqrt{3}}} = 0.15194nm$$

$$\therefore \frac{r_{\min}}{r_{Li}} = 0.225; r_{\min} = 0.414 \times 0.15194nm = 0.06290nm$$

12. The atomic packing fraction for the FCC crystal structure is 0.74. This is the densest arrangement of atoms achievable in three dimensions when all atoms have the same radius *R*. If atoms in the hard sphere model occupy 74% of the volume of the unit cell, then the other 26% is empty space. Imagine that the empty spaces located at the center of each edge and at the body–centered position of the FCC unit cell are filled with smaller spheres of radius *r* such that *r* = 0.414*R*. The smaller atoms fit perfectly in between the atoms of radius *R*. (a) By counting in the usual way, how many atoms of radius *r* are there per FCC unit cell? (b) What are the coordinates of these atoms of radius *r*? Do not double count atoms. Provide the same number of coordinates as the number of atoms of radius *r* per unit cell. (c) What is the atomic packing fraction for this structure?

Solution:

(a)The number of atoms of radius r in per FCC unit cell: $N = \frac{1}{4} \times 8 + 1 = 3$

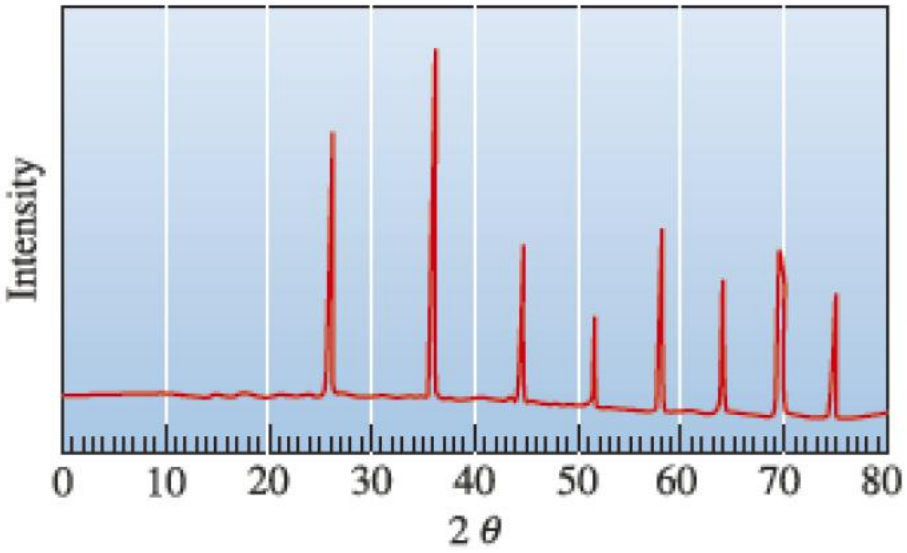
(b)the coordinates of these atoms of radius *r:*

$$\left(\frac{1}{2},0,0\right);\left(0,\frac{1}{2},0\right);\left(1,\frac{1}{2},0\right);\left(\frac{1}{2},1,0\right);\left(\frac{1}{2},0,1\right);\left(0,\frac{1}{2},1\right);\left(1,\frac{1}{2},1\right);\left(\frac{1}{2},1,1\right);\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$$

(c) $$APF = \frac{nV_1}{V} = \frac{4 \times \frac{4}{3}\pi R^3 + 4 \times \frac{4}{3}\pi r^3}{a^3} = \frac{4 \times \frac{4}{3}\pi R^3 + 4 \times \frac{4}{3}\pi (0.414R)^3}{\left(2\sqrt{2}R\right)^3} = 0.78$$

13. The Figure below shows the results of an x-ray diffraction experiment in the form of the intensity of the diffracted peak versus the 2θ diffraction angle. If x-rays with a wavelength of 0.07107 nm are used, determine (a) the crystal structure of the metal; (b) the indices of the planes that produce each of the peaks; and (c) the lattice parameter of the metal.

Solution:???



(a) $\because n\lambda = 2d_{hkl}\sin\theta \therefore d_{hkl} = \dfrac{n\lambda}{2\sin\theta} = \dfrac{0.07107nm}{2\times\sin 13°} = 0.1580nm$

(b)

(c)