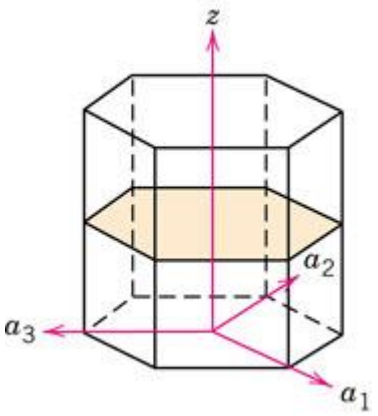
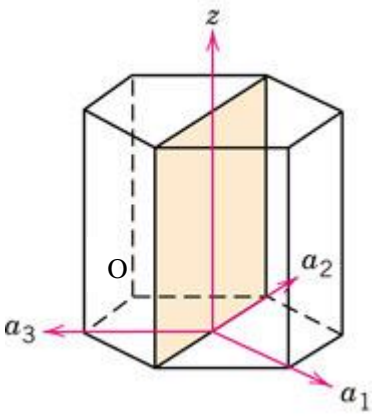
Fundamentals of Materials Science
Homework 9, SS 2017

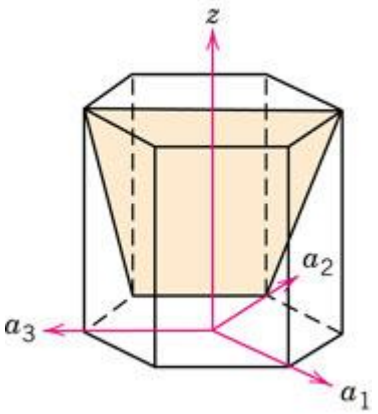
1. Determine the *Miller-Bravais* indices for the planes shown in the following unit cells:



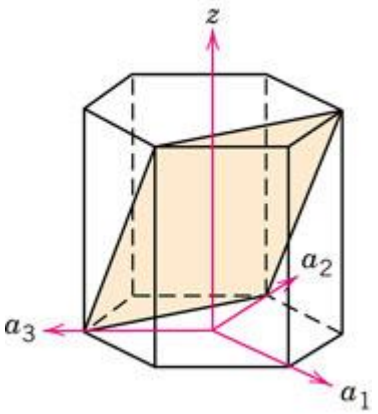
(a)



(b)



(c)



(d)

Solution

(a):

Plane	a_1	a_2	a_3	z
Intercept on axis	$\propto$	$\propto$	$\propto$	$\frac{1}{2}$
Reciprocal of Intercept	0	0	0	2
Enclosure	(0 0 0 2)			

(b): **Define origin as point O**

Plane	a_1	a_2	a_3	z
Intercept on axis	1	$\propto$	-1	$\propto$
Reciprocal of Intercept	1	0	-1	0
Enclosure	(1 0 $\bar{1}$ 0)			

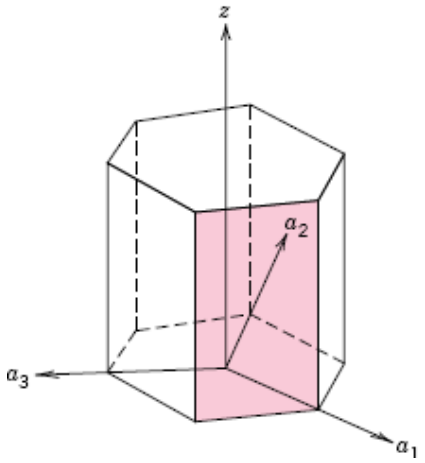
(c):

Plane	a_1	a_2	a_3	z
Intercept on axis	-1	1	∞	1
Reciprocal of Intercept	-1	1	0	1
Enclosure	$(\bar{1}\ 0\ 0\ 1)$			

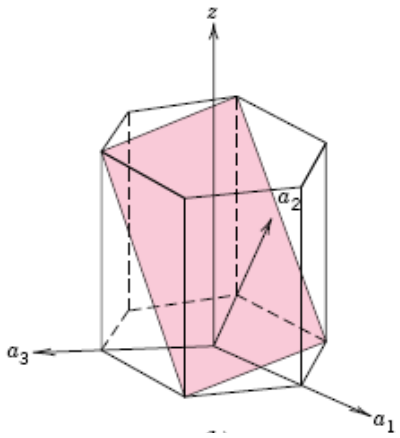
(d):

Plane	a_1	a_2	a_3	z
Intercept on axis	$-\frac{1}{2}$	1	1	$\frac{1}{2}$
Reciprocal of Intercept	-2	1	1	2
Enclosure	$(\bar{2}\ 1\ 1\ 2)$			

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



(a)



(b)

Solotion

(a)

Plane	a_1	a_2	a_3	z
Intercept on axis	1	-1	∞	∞
Reciprocal of Intercept	1	-1	0	0
Enclosure	$(1\ \bar{1}\ 0\ 0)$			

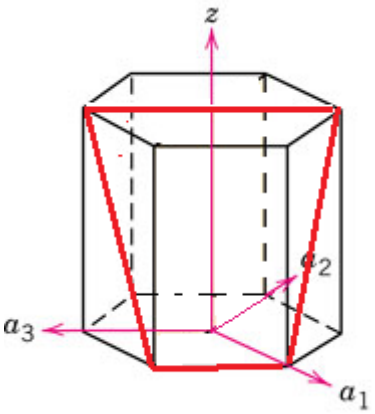
(b)

Plane	a_1	a_2	a_3	z
Intercept on axis	$\frac{1}{2}$	-1	-1	$\frac{1}{2}$
Reciprocal of Intercept	2	-1	-1	2
Enclosure	$(2\ \bar{1}\ \bar{1}\ 2)$			

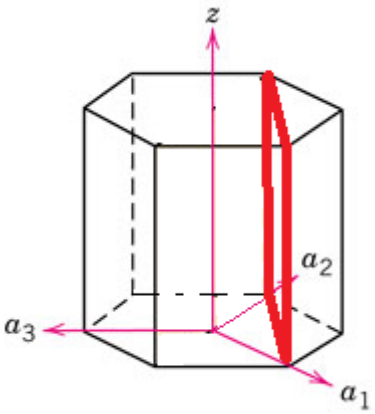
3. Sketch the $(1\ \bar{1}\ 0\ 1)$ and $(11\bar{2}0)$ planes in a hexagonal unit cell.

Solution:

$(1\bar{1}01)$ Plane:



$(11\bar{2}0)$ Plane:



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

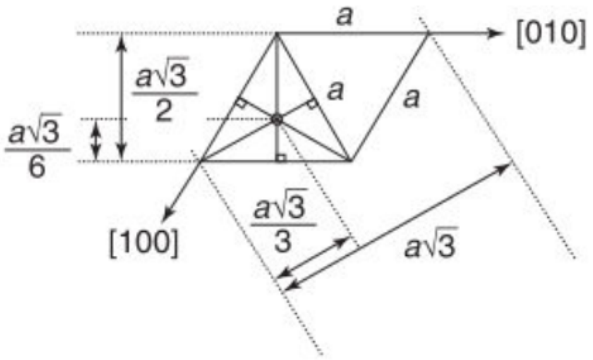
(a) the (100) and (010) planes, [0 1 0]

(b) the (111) and $(11\bar{1})$ planes, $[\bar{1}\ 1\ 0]$

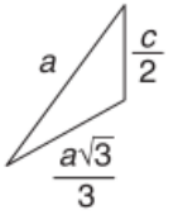
(c) the $(10\bar{1})$ and (001) planes, [1 1 0]

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.

This is an exercise in studying the geometry of the HCP unit cell. The base of the HCP unit cell can be treated as two equilateral triangles each of side a as shown below. The B atom in the HCP structure is located at the (2/3, 1/3, 1/2) location. The distance from the coordinate (1, 0, 0) to (2/3, 1/3, 0), which is the centroid of the triangle in the base, is $\frac{a\sqrt{3}}{3}$.



The *c*/*a* ratio is found by applying the Pythagorean Theorem to the triangle shown below. It is necessary to recognize that each B atom touches the three A atoms in the layer below it at a distance $a = 2R$, where R is the radius of the atom.



$$\left(\frac{a\sqrt{3}}{3}\right)^2 + \left(\frac{c}{2}\right)^2 = a^2$$

Solving for *c*/*a*:

$$\frac{a^2}{3} + \frac{c^2}{4} = a^2$$

$$c^2 = \frac{8a^2}{3}$$

$$\frac{c}{a} = \sqrt{\frac{8}{3}} \blacksquare$$

$$V_C = (\text{AREA})(c) = 6R^2c\sqrt{3}$$

$$= \left(6R^2\sqrt{3}\right)(2)(1.633)R = 12\sqrt{3}\,(1.633)\,R^3$$

Thus,

$$\text{APF} = \frac{V_S}{V_C} = \frac{8\pi R^3}{12\sqrt{3}\,(1.633)\,R^3} = 0.74$$

6. Zirconium has an HCP crystal structure and a density of 6.51 g/cm^3.
   (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*.

(a) The volume of the Zr unit cell may be computed using Equation 4.8 as

$$V_C = \frac{nA_{Zr}}{\rho N_A}$$

Now, for HCP, n = 6 atoms/unit cell, and for Zr, A_{Zr} = 91.22 g/mol. Thus,

$$V_C = \frac{(6 \text{ atoms/unit cell})(91.22 \text{ g/mol})}{(6.51 \text{ g/cm}^3)(6.022 \times 10^{23} \text{ atoms/mol})}$$

$$= 1.396 \times 10^{-22} \text{ cm}^3\text{/unit cell} = 1.396 \times 10^{-28} \text{ m}^3\text{/unit cell}$$

(b) From Equation 4.S1 of the solution to Problem 4.5, for HCP

$$V_C = 6R^2c\sqrt{3}$$

But, since $a = 2R$, (i.e., $R = a/2$) then

$$V_C = 6\left(\frac{a}{2}\right)^2 c\sqrt{3} = \frac{3\sqrt{3}a^2c}{2}$$

but, since $c = 1.593a$

$$V_C = \frac{3\sqrt{3}(1.593)a^3}{2} = 1.396 \times 10^{-22} \text{ cm}^3\text{/unit cell}$$

Now, solving for a

$$a = \left[\frac{(2)(1.396 \times 10^{-22} \text{ cm}^3)}{(3)(\sqrt{3})(1.593)}\right]^{1/3}$$

$$= 3.23 \times 10^{-8} \text{ cm} = 0.323 \text{ nm}$$

And finally

$$c = 1.593a = (1.593)(0.323 \text{ nm}) = 0.515 \text{ nm}$$

7. Rhodium has an atomic radius of 0.1345 nm (1.345Å) and a density of 12.41 g/cm^3. Determine whether it has an FCC or BCC crystal structure.

In order to determine whether Rh has an FCC or a BCC crystal structure, we need to compute its density for each of the crystal structures. For FCC, $n = 4$, and $a = 2R\sqrt{2}$ (Equation 4.1). Also, from Figure 2.8, its atomic weight is 102.91 g/mol. Thus, for FCC (employing Equation 4.8)

$$\rho = \frac{nA_{Rh}}{a^3 N_A} = \frac{nA_{Rh}}{(2R\sqrt{2})^3 N_A}$$

$$= \frac{(4 \text{ atoms/unit cell})(102.91 \text{ g/mol})}{\left\{\left[(2)(1.345 \leftrightarrow 10^{-8} \text{ cm})(\sqrt{2})\right]^3 / (\text{unit cell})\right\}(6.022 \leftrightarrow 10^{23} \text{ atoms/mol})}$$

$$= 12.41 \text{ g/cm}^3$$

which is the value provided in the problem statement. Therefore, Rh has the 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

(a) V(HCP)= $\frac{3\sqrt{3}a}{2} a^2 \times c = \frac{3\sqrt{3}}{2} \times 1.568(2R)^3 = 4.867 \times 10^{-23} cm^3$

(b) p= $\frac{nA}{VNA} = \frac{6 \times 9.012 g/mol}{4.867 \times 10^{23} cm^3 \times 6.02 \times 10^{23} atoms/mol} = 1.845 \text{g}/cm^3$

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)?

$$\text{LD}_{110} = \frac{\text{number of atoms centered on [110] direction vector}}{\text{length of [110] direction vector}}$$

$$= \frac{1 \text{ atom}}{4R\sqrt{\frac{2}{3}}} = \frac{\sqrt{3}}{4R\sqrt{2}}$$

$$\mathrm{LD}_{111} = \frac{\text{number of atoms centered on [111] direction vector}}{\text{length of [111] direction vector}}$$

$$= \frac{2 \text{ atoms}}{4R} = \frac{1}{2R}$$

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)?

$$\mathrm{LD}_{100} = \frac{\text{number of atoms centered on [100] direction vector}}{\text{length of [100] direction vector}}$$

$$= \frac{1 \text{ atom}}{2R\sqrt{2}} = \frac{1}{2R\sqrt{2}}$$

$$\mathrm{LD}_{111} = \frac{\text{number of atoms centered on [111] direction vector}}{\text{length of [111] direction vector}}$$

$$= \frac{1 \text{ atom}}{2R\sqrt{6}} = \frac{1}{2R\sqrt{6}}$$

11. 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_{111} thick is the sheet? See Appendices in your textbook for necessary data.

$$d_{111} = \frac{a_0}{\sqrt{1^2 + 1^2 + 1^2}} = \frac{3.796 \text{ Å}}{\sqrt{3}} = 2.1916 \text{ Å}$$

$$\text{thickness} = \frac{0.1 \text{ mm}}{2.1916 \times 10^{-8} \text{ cm}} = \boxed{4.563 \times 10^6 \times d_{111}}$$

12. 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.

For the tetrahedral site in FCC nickel (a_0 = 3.5167 Å):

$$r_{\mathrm{Ni}} = \frac{\sqrt{2}}{4}(3.5167\ \text{Å}) = 1.2433\ \text{Å}$$

$$\left(\frac{r}{r_{\mathrm{Ni}}}\right)_{\text{tetrahedral site}} = 0.225$$

$$r = (1.2433\ \text{Å})(0.225)$$

$$\boxed{r = 0.2798\ \text{Å}}$$

For the octahedral site in BCC lithium (a_0 = 3.5089 Å):

$$r_{\mathrm{Li}} = \frac{\sqrt{3}}{4}(3.5089\ \text{Å}) = 1.519\ \text{Å}$$

$$\left(\frac{r}{r_{\mathrm{Li}}}\right)_{\text{octahedral site}} = 0.414$$

$$r = (3.5089\ \text{Å})(0.414)$$

$$\boxed{r = 0.6290\ \text{Å}}$$

13. 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 $r = 0.414R$. 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:

$$\frac{1}{4}\frac{\text{atom}}{\text{edge}} * 12 \text{ edges} + 1 \text{ body–center} = 4 \text{ atoms of radius } r$$

These atoms have the following coordinates:

(½ , 0, 0) (0, ½ , 0) (0, 0, ½) (½, ½, ½)

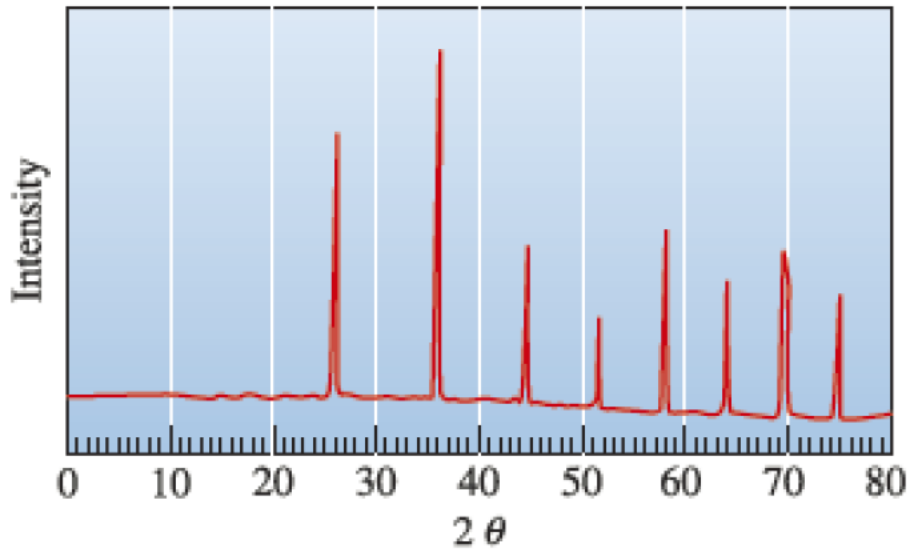
By definition, the APF is

$$\text{APF} = \frac{\text{number of atoms per unit cell} * \text{atomic volume}}{\text{unit cell volume}}$$

There are four atoms per unit cell with radius *R* and four atoms per unit cell with radius *r*. Since the smaller atoms fit perfectly in between the atoms of radius *R*, $a\sqrt{2} = 4R$, where *a* is the lattice parameter for the FCC unit cell.

$$\text{APF} = \frac{4 * \frac{4}{3}\pi R^3 + 4 * \frac{4}{3}\pi r^3}{(4R/\sqrt{2})^3} = \frac{4 * \frac{4}{3}\pi R^3 + 4 * \frac{4}{3}\pi (0.414R)^3}{(4R/\sqrt{2})^3} = \frac{\frac{16}{3}\pi + \frac{16}{3}\pi (0.414)^3}{(4/\sqrt{2})^3} = 0.79$$

14. 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.



The 2ϑ values can be estimated from the figure:

	2ϑ	$\sin^2\vartheta$	$\sin^2\vartheta/0.0077$	Planar indicies	$d = \lambda/(2\sin\vartheta)$	$a_0 = (h^2 + k^2 + l^2)^{0.5}$
1	25.5	0.049	1	(110)	0.1624	0.2297
2	36.5	0.095	2	(200)	0.116	0.2320
3	44.5	0.143	3	(211)	0.0947	0.2319
4	51.5	0.189	4	(220)	0.0825	0.2334
5	58.5	0.235	5	(310)	0.0739	0.2338
6	64.5	0.285	6	(222)	0.0672	0.2327
7	70.5	0.329	7	(321)	0.0625	0.2339
8	75.5	0.375	8	(400)	0.0586	0.2342

The sequence 1, 2, 3, 4, 5, 6, 7, 8 (which includes the "7") means that the material is BCC.

The average a_0 = 0.2327 nm.