Note: These questions will be discussed in the tutorial sessions on September 26.

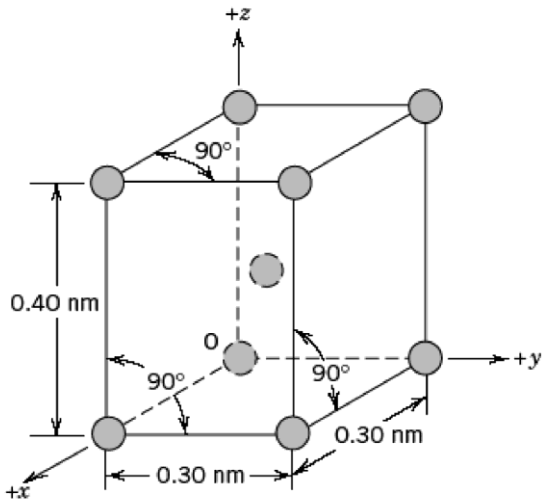
Question 1:

Below is a unit cell for a hypothetical metal.

(a) To which crystal system does this unit cell belong?

(b) What would this crystal structure be called?

(c) Calculate the density of the material, given that its atomic weight is 141 g/mol.



Solution:

(a) The unit cell shown in the problem statement belongs to the tetragonal crystal system since $a = b = 0.30$ nm, $c = 0.40$ nm, and $\alpha = \beta = \gamma = 90°$.

(b) The crystal structure would be called *body-centered tetragonal*.

(c) As with BCC, $n = 2$ atoms/unit cell. Also, for this unit cell

$$V_C = (3.0 \times 10^{-8}\ \text{cm})^2(4.0 \times 10^{-8}\ \text{cm})$$

$$= 3.60 \times 10^{-23}\ \text{cm}^3/\text{unit cell}$$

Thus, using Equation 3.5, the density is equal to

$$\rho = \frac{nA}{V_C N_A}$$

$$= \frac{(2\ \text{atoms/unit cell})(141\ \text{g/mol})}{(3.60 \times 10^{-23}\ \text{cm}^3/\text{unit cell})(6.022 \times 10^{23}\ \text{atoms/mol})}$$

= 13.0 g/cm3

Question 2:

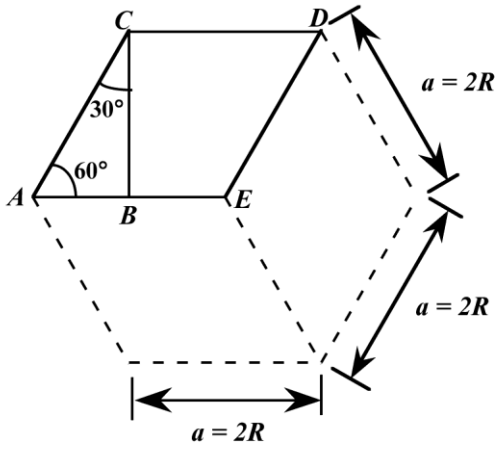
Show that the atomic packing factor for HCP is 0.74.

Solution:

The APF is just the total sphere volume-unit cell volume ratio. For HCP, there are the equivalent of six spheres per unit cell, and thus

$$V_S = 6\left(\frac{4\pi R^3}{3}\right) = 8\pi R^3$$

Now, the unit cell volume is just the product of the base area times the cell height, *c*. This base area is just three times the area of the parallelepiped *ACDE* shown below.



The area of *ACDE* is just the length of $\overline{CD}$ times the height $\overline{BC}$. But $\overline{CD}$ is just *a* or 2*R*, and

$$\overline{BC} = 2R\cos(30°) = \frac{2R\sqrt{3}}{2}$$

Thus, the base area is just

$$\text{AREA} = (3)(\overline{CD})(\overline{BC}) = (3)(2R)\left(\frac{2R\sqrt{3}}{2}\right) = 6R^2\sqrt{3}$$

and since $c = 1.633a = 2R(1.633)$

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

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

Thus,

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

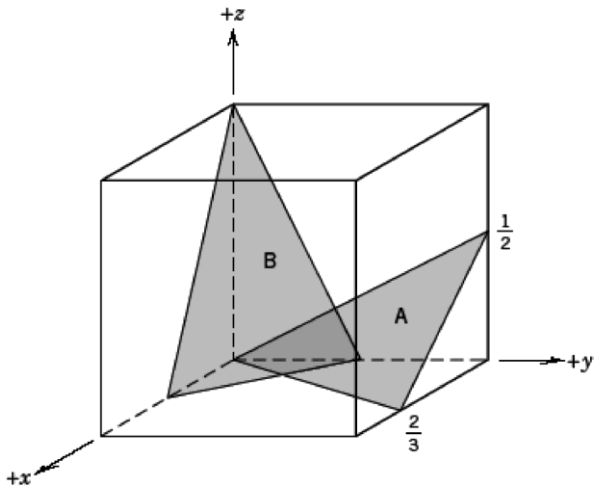
Question 3:

a) Sketch a tetragonal unit cell, and within that cell indicate locations of the $\frac{1}{2}\,1\,\frac{1}{2}$ and $\frac{1}{4}\,\frac{1}{2}\,\frac{3}{4}$ point coordinates.

b) Within a cubic unit cell, sketch the following directions:

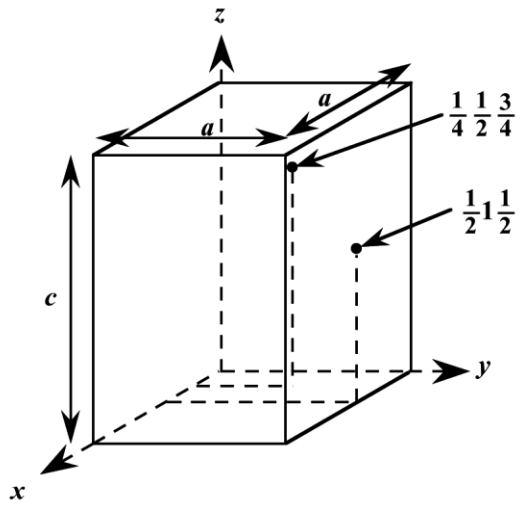
$[\bar{1}10]$, $[\bar{1}\bar{2}1]$, $[0\bar{1}2]$

c) Determine the Miller indices for the planes shown in the following unit cell:

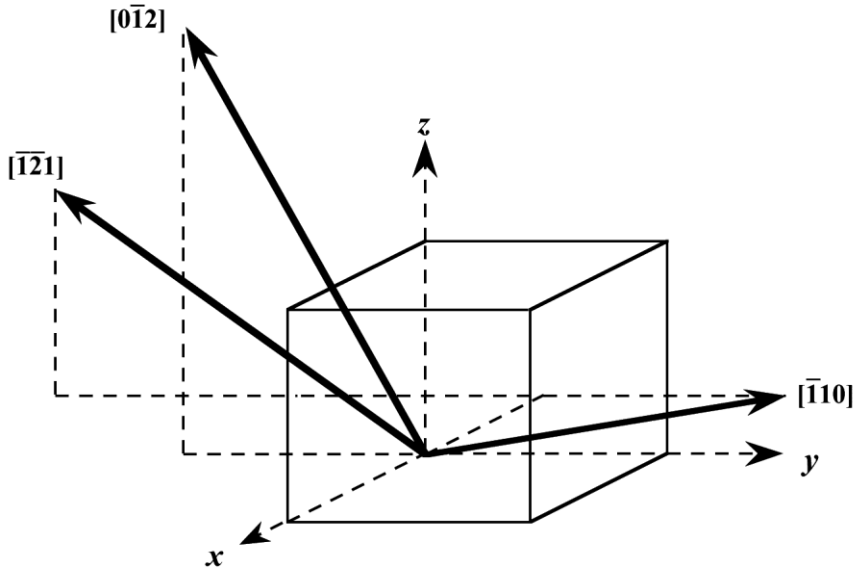


Solution:

a) A tetragonal unit in which are shown the $\frac{1}{2}\,1\,\frac{1}{2}$ and $\frac{1}{4}\,\frac{1}{2}\,\frac{3}{4}$ point coordinates is presented below.



b) The directions asked for are indicated in the cubic unit cells shown below.



c) For plane A since the plane passes through the origin of the coordinate system as shown, we will move the origin of the coordinate system one unit cell distance to the right along the *y* axis; thus, this is a $(3\bar{2}4)$ plane, as summarized below.

	x	y	z
Intercepts	$\frac{2a}{3}$	$-b$	$\frac{c}{2}$
Intercepts in terms of *a*, *b*, and *c*	$\frac{2}{3}$	-1	$\frac{1}{2}$
Reciprocals of intercepts	$\frac{3}{2}$	-1	2
Reduction	3	-2	4
Enclosure		$(3\bar{2}4)$	

For plane B we will leave the origin at the unit cell as shown; this is a (221) plane, as summarized below.

	x	y	z
Intercepts	$\frac{a}{2}$	$\frac{b}{2}$	*c*
Intercepts in terms of *a*, *b*, and *c*	$\frac{1}{2}$	$\frac{1}{2}$	1
Reciprocals of intercepts	2	2	1

Reduction	not necessary
Enclosure	(221)

Question 4:

Determine the expected diffraction angle for the first-order reflection from the (113) set of planes for FCC platinum when monochromatic radiation of wavelength 0.1542 nm is used.

Solution:

We first calculate the lattice parameter using Equation 3.1 and the value of R (0.1387 nm) cited in Table 3.1, as follows:

$$a = 2R\sqrt{2} = (2)(0.1387\ \text{nm})(\sqrt{2}) = 0.3923\ \ \text{nm}$$

Next, the interplanar spacing for the (113) set of planes may be determined using Equation 3.14 according to

$$d_{113} = \frac{a}{\sqrt{(1)^2 + (1)^2 + (3)^2}} = \frac{0.3923\ \text{nm}}{\sqrt{11}} = 0.1183\ \ \text{nm}$$

And finally, employment of Equation 3.13 yields the diffraction angle as

$$\sin\theta = \frac{n\lambda}{2d_{113}} = \frac{(1)(0.1542\ \text{nm})}{(2)(0.1183\ \text{nm})} = 0.652$$

Which leads to

$$\theta = \sin^{-1}(0.652) = 40.69°$$

And, finally

$$2\theta = (2)(40.69°) = 81.38°$$

Question 5:

What is the composition, in atom percent, of an alloy that contains 99.7 lb_m copper, 102 lb_m zinc, and 2.1 lb_m lead?

Solution:

In this problem we are asked to determine the concentrations, in atom percent, of the Cu-Zn-Pb alloy. It is first necessary to convert the amounts of Cu, Zn, and Pb into grams.

$$m'_{Cu} = (99.7\ \text{lb}_m)(453.6\ \text{g/lb}_m) = 45{,}224\ \text{g}$$

$$m'_{Zn} = (102\ \text{lb}_m)(453.6\ \text{g/lb}_m) = 46{,}267\ \text{g}$$

$$m'_{Pb} = (2.1\ lb_m)(453.6\ g/lb_m) = 953\ g$$

These masses must next be converted into moles (Equation 4.4), as

$$n_{m_{Cu}} = \frac{m'_{Cu}}{A_{Cu}} = \frac{45,224\ g}{63.55\ g/mol} = 711.6\ mol$$

$$n_{m_{Zn}} = \frac{46,267\ g}{65.41\ g/mol} = 707.3\ mol$$

$$n_{m_{Pb}} = \frac{953\ g}{207.2\ g/mol} = 4.6\ mol$$

Now, employment of a modified form of Equation 4.5, gives

$$C'_{Cu} = \frac{n_{m_{Cu}}}{n_{m_{Cu}} + n_{m_{Zn}} + n_{m_{Pb}}} \times 100$$

$$= \frac{711.6\ mol}{711.6\ mol + 707.3\ mol + 4.6\ mol} \times 100 = 50.0\ at\%$$

$$C'_{Zn} = \frac{707.3\ mol}{711.6\ mol + 707.3\ mol + 4.6\ mol} \times 100 = 49.7\ at\%$$

$$C'_{Pb} = \frac{4.6\ mol}{711.6\ mol + 707.3\ mol + 4.6\ mol} \times 100 = 0.3\ at\%$$

Question 6:

For a BCC single crystal, would you expect the surface energy for a (100) plane to be greater or less than that for a (110) plane? Why?

Solution:

The surface energy for a crystallographic plane will depend on its packing density [i.e., the planar density (Section 3.11)]—that is, the higher the packing density, the greater the number of nearest-neighbor atoms, and the more atomic bonds in that plane that are satisfied, and, consequently, the lower the surface energy. From the solution to Problem 3.55, the planar densities for BCC (100) and (110) are $\frac{3}{16R^2}$ and $\frac{3}{8R^2\sqrt{2}}$, respectively—that is $\frac{0.19}{R^2}$ and $\frac{0.27}{R^2}$. Thus, since the planar density for (110) is greater, it will have the lower surface energy.