

**MAE 20
Winter 2011
Assignment 1 solutions**

1.

2.8 The K^+ ion is just a potassium atom that has lost one electron; therefore, it has an electron configuration the same as argon (Figure 2.6).

The I^- ion is a iodine atom that has acquired one extra electron; therefore, it has an electron configuration the same as xenon.

2.

2.13 The attractive force between two ions F_A is just the derivative with respect to the interatomic separation of the attractive energy expression, Equation 2.8, which is just

$$F_A = \frac{dE_A}{dr} = \frac{d\left(-\frac{A}{r}\right)}{dr} = \frac{A}{r^2}$$

The constant A in this expression is defined in footnote 3. Since the valences of the Ca^{2+} and O^{2-} ions (Z_1 and Z_2) are both 2, then

$$\begin{aligned} F_A &= \frac{(Z_1 e)(Z_2 e)}{4\pi\epsilon_0 r^2} \\ &= \frac{(2)(2)(1.6 \times 10^{-19} \text{ C})^2}{(4)(\pi)(8.85 \times 10^{-12} \text{ F/m})(1.25 \times 10^{-9} \text{ m})^2} \\ &= 5.89 \times 10^{-10} \text{ N} \end{aligned}$$

3.

2.14 (a) Differentiation of Equation 2.11 yields

$$\begin{aligned}\frac{dE_N}{dr} &= \frac{d\left(-\frac{A}{r}\right)}{dr} + \frac{d\left(\frac{B}{r^n}\right)}{dr} \\ &= \frac{A}{r^{(1+1)}} - \frac{nB}{r^{(n+1)}} = 0\end{aligned}$$

(b) Now, solving for r ($= r_0$)

$$\frac{A}{r_0^2} = \frac{nB}{r_0^{(n+1)}}$$

or

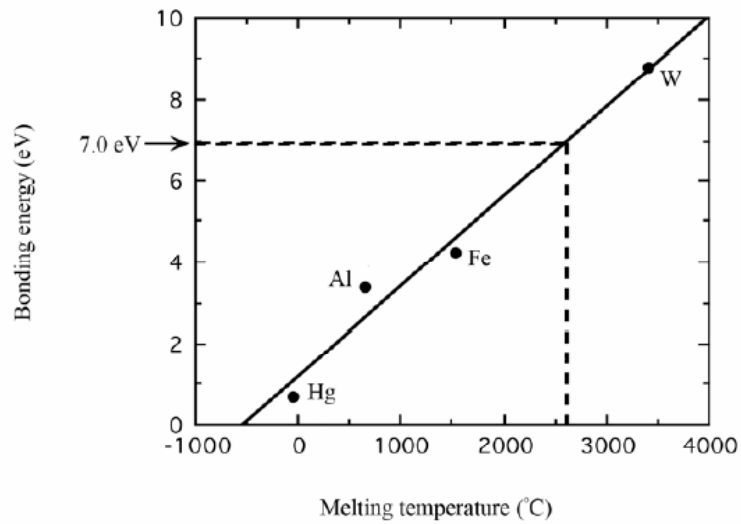
$$r_0 = \left(\frac{A}{nB}\right)^{1/(1-n)}$$

(c) Substitution for r_0 into Equation 2.11 and solving for E ($= E_0$)

$$\begin{aligned}E_0 &= -\frac{A}{r_0} + \frac{B}{r_0^n} \\ &= -\frac{A}{\left(\frac{A}{nB}\right)^{1/(1-n)}} + \frac{B}{\left(\frac{A}{nB}\right)^{n/(1-n)}}\end{aligned}$$

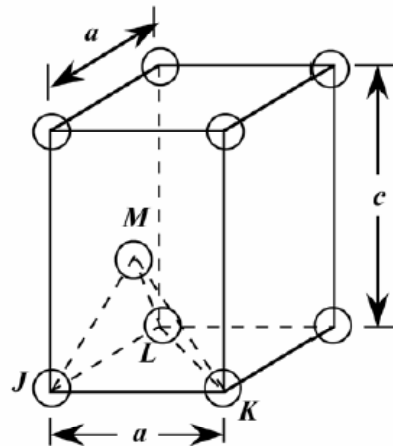
4.

2.20 Below is plotted the bonding energy versus melting temperature for these four metals. From this plot, the bonding energy for molybdenum (melting temperature of 2617°C) should be approximately 7.0 eV. The experimental value is 6.8 eV.

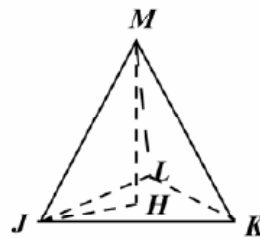


5.

3.4 We are asked to show that the ideal c/a ratio for HCP is 1.633. A sketch of one-third of an HCP unit cell is shown below.



Consider the tetrahedron labeled as $JKLM$, which is reconstructed as



The atom at point M is midway between the top and bottom faces of the unit cell--that is $\overline{MH} = c/2$. And, since atoms at points J , K , and M , all touch one another,

$$\overline{JM} = \overline{JK} = 2R = a$$

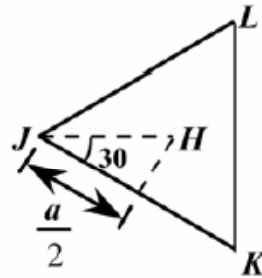
where R is the atomic radius. Furthermore, from triangle JHM ,

$$(\overline{JM})^2 = (\overline{JH})^2 + (\overline{MH})^2$$

or

$$a^2 = (\overline{JH})^2 + \left(\frac{c}{2}\right)^2$$

Now, we can determine the \overline{JH} length by consideration of triangle JKL , which is an equilateral triangle.



$$\cos 30^\circ = \frac{a/2}{\overline{JH}} = \frac{\sqrt{3}}{2}$$

and

$$\overline{JH} = \frac{a}{\sqrt{3}}$$

Substituting this value for \overline{JH} in the above expression yields

$$a^2 = \left(\frac{a}{\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2 = \frac{a^2}{3} + \frac{c^2}{4}$$

and, solving for c/a

$$\frac{c}{a} = \sqrt{\frac{8}{3}} = 1.633$$

6.

3.5 We are asked to show that the atomic packing factor for BCC is 0.68. The atomic packing factor defined as the ratio of sphere volume to the total unit cell volume, or

$$\text{APF} = \frac{V_S}{V_C}$$

Since there are two spheres associated with each unit cell for BCC

$$V_S = 2(\text{sphere volume}) = 2\left(\frac{4\pi R^3}{3}\right) = \frac{8\pi R^3}{3}$$

Also, the unit cell has cubic symmetry, that is $V_C = a^3$. But a depends on R according to Equation 3.3, and

$$V_C = \left(\frac{4R}{\sqrt{3}}\right)^3 = \frac{64R^3}{3\sqrt{3}}$$

Thus,

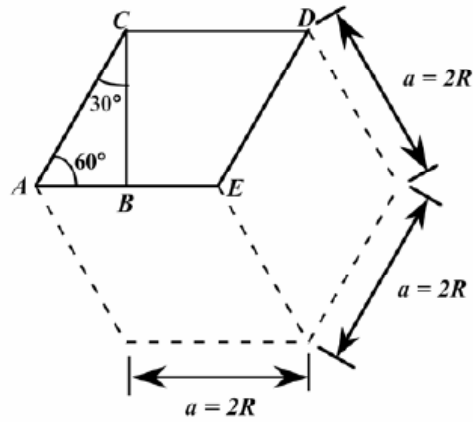
$$\text{APF} = \frac{V_S}{V_C} = \frac{8\pi R^3/3}{64R^3/3\sqrt{3}} = 0.68$$

7.

3.6 This problem calls for a demonstration that the APF for HCP is 0.74. Again, the APF is just the 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 $2R$, and

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

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

$$V_C = (\text{AREA})(c) = 6R^2c\sqrt{3} = (6R^2\sqrt{3})(2)(1.633)R = 12\sqrt{3}(1.633)R^3$$

Thus,

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

8.

3.8 We are asked to determine the radius of a palladium atom, given that Pd has an FCC crystal structure. For FCC, $n = 4$ atoms/unit cell, and $V_C = 16R^3\sqrt{2}$ (Equation 3.4). Now,

$$\begin{aligned}\rho &= \frac{nA_{\text{Pd}}}{V_C N_A} \\ &= \frac{nA_{\text{Pd}}}{(16R^3\sqrt{2})N_A}\end{aligned}$$

And solving for R from the above expression yields

$$\begin{aligned}R &= \left(\frac{nA_{\text{Pd}}}{16\rho N_A \sqrt{2}} \right)^{1/3} \\ &= \left[\frac{(4 \text{ atoms/unit cell})(106.4 \text{ g/mol})}{(16)(12.0 \text{ g/cm}^3)(6.023 \times 10^{23} \text{ atoms/mol})(\sqrt{2})} \right]^{1/3} \\ &= 1.38 \times 10^{-8} \text{ cm} = 0.138 \text{ nm}\end{aligned}$$

9.

3.14 For each of these three alloys we need, by trial and error, to calculate the density using Equation 3.5 and compare it to the value cited in the problem. For SC, BCC, and FCC crystal structures, the respective values of n are 1, 2, and 4, whereas the expressions for a (since $V_C = a^3$) are $2R$, $2R\sqrt{2}$, and $\frac{4R}{\sqrt{3}}$.

For alloy A, let us calculate ρ assuming a BCC crystal structure.

$$\begin{aligned}\rho &= \frac{nA_A}{V_C N_A} \\ &= \frac{nA_A}{\left(\frac{4R}{\sqrt{3}}\right)^3 N_A} \\ &= \frac{(2 \text{ atoms/unit cell})(43.1 \text{ g/mol})}{\left\{ \left[\frac{(4)(1.22 \times 10^{-8} \text{ cm})}{\sqrt{3}} \right]^3 / (\text{unit cell}) \right\} (6.023 \times 10^{23} \text{ atoms/mol})} \\ &= 6.40 \text{ g/cm}^3\end{aligned}$$

Therefore, its crystal structure is BCC.

For alloy B, let us calculate ρ assuming a simple cubic crystal structure.

$$\begin{aligned}\rho &= \frac{nA_B}{(2a)^3 N_A} \\ &= \frac{(1 \text{ atom/unit cell})(184.4 \text{ g/mol})}{\left\{ \left[(2)(1.46 \times 10^{-8} \text{ cm}) \right]^3 / (\text{unit cell}) \right\} (6.023 \times 10^{23} \text{ atoms/mol})} \\ &= 12.3 \text{ g/cm}^3\end{aligned}$$

Therefore, its crystal structure is simple cubic.

For alloy C, let us calculate ρ assuming a BCC crystal structure.

$$\rho = \frac{nA_C}{\left(\frac{4R}{\sqrt{3}}\right)^3 N_A}$$

$$= \frac{(2 \text{ atoms/unit cell})(91.6 \text{ g/mol})}{\left\{ \left[\frac{(4)(1.37 \times 10^{-8} \text{ cm})}{\sqrt{3}} \right]^3 / (\text{unit cell}) \right\} (6.023 \times 10^{23} \text{ atoms/mol})}$$

$$= 9.60 \text{ g/cm}^3$$

Therefore, its crystal structure is BCC.