HW A

Problem 2.14

a. To Find:

The bond energy between two ions (E_O) expressed as a function of three parameters A, B and n.

b. Given:

The equation representing variation of the net potential energy between two adjacent ions (E_N) with inter-ionic spacing (r) :

$$E_N = -\frac{A}{r} + \frac{B}{r^n} \qquad (\ldots 1)$$

c. Assumptions: None Obvious

d. Solution:

(1) Differentiating the given equation, we get:

$$\frac{dE_N}{dr} = \frac{d\left(-\frac{A}{r}\right)}{dr} + \frac{d\left(\frac{B}{r^n}\right)}{dr} \qquad (\ldots 2)$$

$$\Rightarrow \quad \frac{dE_N}{dr} = \frac{A}{r^{(1+1)}} - \frac{nB}{r^{(n+1)}} \qquad (\ldots 3)$$

The minimum in the E vs r curve occurs when

$$\frac{dE_N}{dr} = 0$$

$$\Rightarrow \quad \frac{A}{r^{(2)}} - \frac{nB}{r^{(n+1)}} = 0$$

$$\Rightarrow \quad \frac{A}{r^{(2)}} = \frac{nB}{r^{(n+1)}} \qquad (\ldots 4)$$

(2) This minimum in the E vs r curve occurs when r=r_o **.** Solving for r_o:

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

(In the above equation ro = r_o)

$$\Rightarrow r_o = \left(\frac{A}{nB}\right)^{1/(1-n)} \qquad (\ldots 5)$$

(3) $E_N = E_o$ when r = r_o.

$$E_0 = -\frac{A}{r_o} + \frac{B}{r_o^n}$$

From equation (…5)

$$\mathrm{Eo} = -\frac{A}{\left(\frac{A}{nB}\right)^{1/(1-n)}} + \frac{B}{\left(\frac{A}{nB}\right)^{n/(1-n)}} \qquad (\ldots 6)$$

Problem 2.15

a. To Find:

Whether graphically obtained and mathematically calculated values of E_o are equal. Also, whether graphically obtained and mathematically calculated values of r_o are equal.

b. Given:

$$E_A = -\frac{1.436}{r}$$

$$E_R = \frac{5.8 \times 10^{-6}}{r^9}$$

$E_N = E_A + E_R$

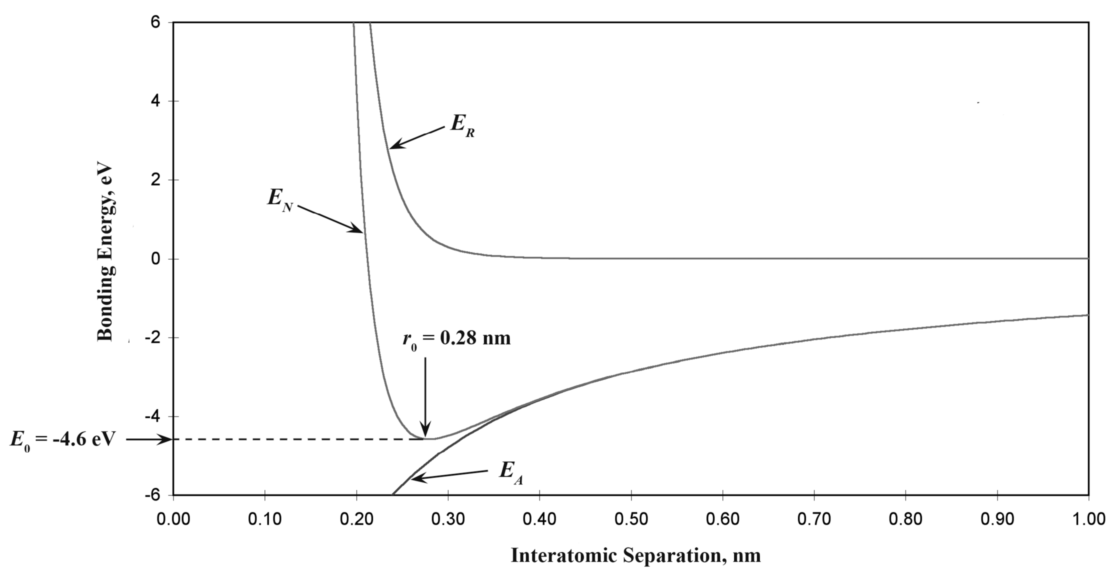
c. Assumptions:

(i) Sufficient values of 'r' considered so as to ensure accuracy in plotting the curves and obtaining correct values for E_o and r_o.

(ii) The given expressions for E_A and E_R are accurate representations of the interaction between K^+ and Cl^-.

d. Solution:

(a) Curves of E_A, E_R, and E_N vs r



(b) From the E_N vs r plot:

(1) r_o = r co-ordinate of minimum of plot = 0.28 nm
(2) E_o = E co-ordinate of minimum of plot = -4.6 eV

(c) Comparing equations for E_N in Prob. 2.14 and Prob. 2.15

A = 1.436

B = 5.86 X 10^{-6}

n = 9

From Prob. 2.14

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

⇨ $$r_o = \left[\frac{1.436}{(9)(5.86\times10^{-6})}\right]^{1/(1-9)}$$

⇨

⇨ $$\boxed{ro = 0.279\,\text{nm}}$$ (Here ro = r_o)

From Prob. 2.14

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

⇨

$$Eo = -\frac{1.436}{\left[\frac{1.436}{(9)(5.86\times10^{-6})}\right]^{1/(1-9)}} + \frac{5.86\times10^{-6}}{\left[\frac{1.436}{(9)(5.86\times10^{-6})}\right]^{9/(1-9)}}$$

$$\boxed{Eo = -4.57\,\text{eV}}$$

Problem 2.20

a. To Find:

To plot bonding energy vs. melting temperature and point out the approximate position of copper on this plot

b. Given:

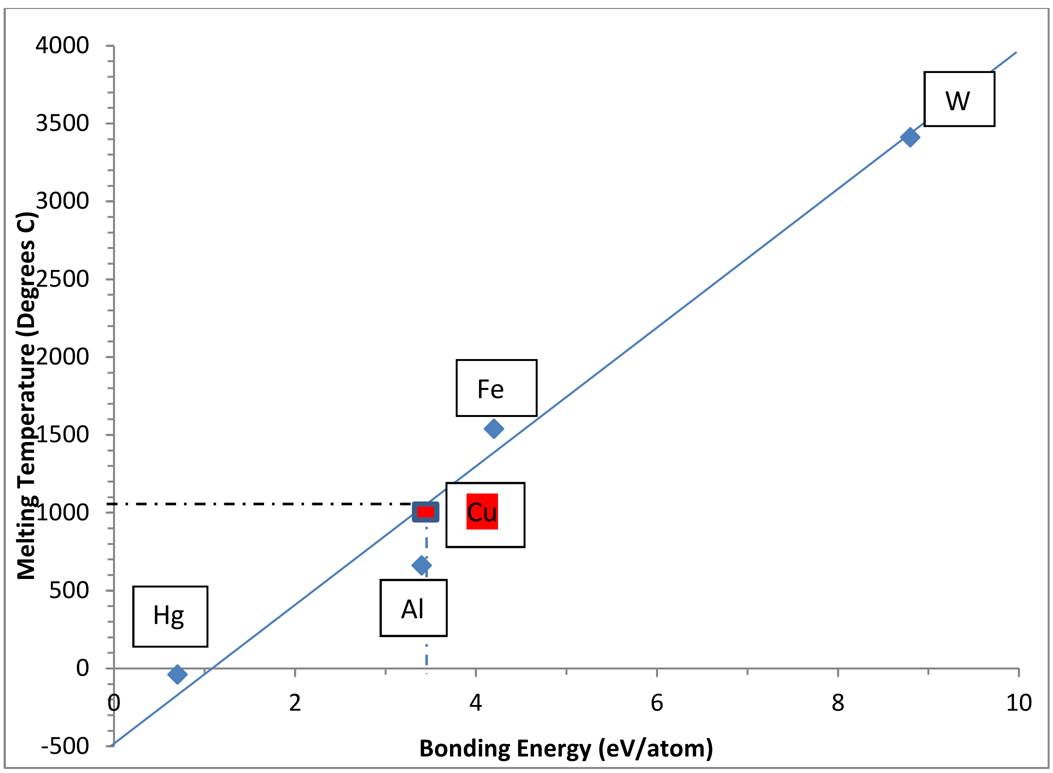
Bonding energies and melting temperatures of various metals.

c. Assumptions:

Linear trend/ linear relationship between bonding energy and melting temperature for the four metals under consideration. We overlook minor deviations from the straight line. Doing this will enable us to locate the position of copper on this plot.

This assumption also suggests that melting temperature is primarily determined by bonding energy and that other factors are small, secondary or tertiary, for e.g., grain sie or defect concentration.

d. Solution:



Plot of Bonding Energy vs. Melting Temperature

Depending on how we draw the straight line, there are a range of answers possible. For e.g., the best fit line connecting the points corresponding to Hg, Fe and W, yields an answer of 3.3 eV.

From this particular plot, the bonding energy for copper (melting temperature of 1084°C) should be approximately 3.6 eV.

Bonding energy of copper ≈ 3.6 eV

Problem 3.7

a. To Find:

Theoretical density for iron. Also, comparison of experimental density with theoretical density.

b. Given:

Crystal Structure of iron = BCC

Atomic radius, R = 0.124 nm

Atomic weight, A_{Fe} = 55.85 g/ml

c. Assumptions:

(i) Hard sphere model of atom
(ii) Perfect crystal / No defects in crystal

d. Solution:

From equation 3.5:

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

For BCC, n = 2 atoms/unit cell

Let 'a' be the edge of the unit cell. For BCC:

$$a = \left(\frac{4R}{\sqrt{3}}\right)$$

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

Thus,

$$\rho = \frac{nA_{\mathrm{Fe}}}{\left(\frac{4\,R}{\sqrt{3}}\right)^3 N_{\mathrm{A}}}$$

$$\rho = \frac{(2 \text{ atoms/unit cell})(55.85 \text{ g/mol})}{\left[(4)\left(0.124 \times 10^{-7} \text{ cm}\right)/\sqrt{3}\right]^3 /(\text{unit cell})\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}$$

ρ = 7.90 g/cm^3

The theoretical density is very close to the experimental value of 7.87 g/cm^3.

Problem 3.17

a. To Find:

Theoretical density for titanium. Also, comparison of experimental density with theoretical density.

b. Given:

Crystal structure of Titanium = HCP

Atomic radius, R = 0.1445 nm

c/a = 1.58

c. Assumptions:

(iii) Hard sphere model of atom
(iv) Perfect crystal / No defects in crystal

d. Solution:

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

For HCP, n = 6

A_{Ti} = 47.87 g/mol (as noted inside the front cover)

Let the edge of the hexagon have a length 'a'.

Then, $Vc = 6 * \frac{\sqrt{3}}{4} * a^2 * c$
Since, a = 2*R

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

For c/a = 1.58 =>c/(2*R) = 1.58 => c/R = 3.16

$$V_C = (6)(3.16)R^3\sqrt{3}$$
$$V_C = (6)(3.16)(\sqrt{3})\left[1.445 \times 10^{-8} \text{ cm}\right]^3$$
$$V_C = 9.91 \times 10^{-23} \text{ cm}^3\text{/unit cell}$$

$$\rho = \frac{(6\ \text{atoms/unit cell})(47.87\ \text{g/mol})}{\left(9.91 \times 10^{-23}\ \text{cm}^3\text{/unit cell}\right)\left(6.022 \times 10^{23}\ \text{atoms/mol}\right)}$$

$$\boldsymbol{\rho = 4.81\ \text{g/cm}^3}$$

The value given in the literature is 4.51 g/cm^3