Homework 4 Solutions.

Chapter 3:

(3) FOR FCC

$$U = -(2.15)(4N\varepsilon)$$

FOR 1 MOLE, $N = 6.02 \times 10^{23}$
AND IF $\varepsilon = 50 \times 10^{-16}$ ERG,

$$U = -(2.15)(4)(6.02 \times 10^{23})(50 \times 10^{-16}\ \text{ERG})$$

$$= 2.59 \times 10^{10}\ \text{ERG/MOLE} = \boxed{2.59\ \frac{\text{kJ}}{\text{MOLE}} = U}$$

(5) THE PAIR POTENTIAL CAN BE WRITTEN

$$U_{ij}(R_{ij}) = \begin{cases} \dfrac{A}{R_{ij}^{n}} - \dfrac{q^2}{R_{ij}} & ij \text{ ARE NEAREST NEIGHBOR} \\[2ex] \pm \dfrac{q^2}{R_{ij}} & i, j \text{ NOT NEAREST NEIGHBORS} \end{cases}$$

LET R = NEAREST NEIGHBOR DISTANCE SO THAT

$$R_{ij} = p_{ij} R. \qquad \text{THEN}$$

$$U_{ij}(R) = \begin{cases} \dfrac{A}{R^n} - \dfrac{q^2}{R} & i,j \text{ (NEAREST NEIGHBORS)} \\ \pm \dfrac{q^2}{p_{ij} R} & i,j \text{ NOT NEAREST NEIGHBORS} \end{cases}$$

THE TOTAL ENERGY IS

$$U = \frac{2N}{2}\left({\sum_j}' \frac{\pm q^2}{p_{ij} R} \right) + N \frac{A}{R^n}$$

$$U = N\left(\frac{A}{R^n} - \frac{q^2}{R} {\sum_j}' \frac{\pm 1}{p_{ij}} \right)$$

$$= N\left(\frac{A}{R^n} - \frac{q^2}{R}\left(2 \ln 2\right) \right)$$

(WE APPROXIMATE ${\sum_j}'$ AS AN INFINITE SUM) $\left(\sum_{i=1}^{\infty} \frac{(-1)^{i+1}}{i} = \ln 2 \right)$

AT EQ. $\left.\dfrac{\partial U}{\partial R}\right|_{R_0} = 0, \Rightarrow$

$$-\frac{nA}{R_0^{n+1}} + \frac{q^2}{R_0^2}\, 2\ln 2 = 0$$

$$\Rightarrow R_0^{n-1} = \frac{nA}{q^2\, 2\ln 2} \Rightarrow \frac{q^2}{R_0} 2\ln 2 = \frac{nA}{R_0^n}$$

so

$$U = N\left(\frac{q^2\, 2\ln 2}{n R_0} - \frac{q^2\, 2\ln 2}{R_0}\right)$$

or

$$\boxed{U(R_0) = -\frac{N q^2\, 2\ln 2}{R_0}\left(1 - \frac{1}{n}\right)}$$

(B) $$U(R_0(1-\delta)) = U(R_0) + \frac{1}{2}\left.\frac{\partial^2 U}{\partial R^2}\right|_{R_0} (R_0\delta)^2 + \ldots$$

FOR UNIT LENGTH, $2NR_0 = 1$.

NOW $$\left.\frac{\partial^2 U}{\partial R^2}\right|_{R_0} = N\left(\frac{n(n+1)A}{R_0^{n+2}} - \frac{2(2\ln 2)q^2}{R_0^3}\right)$$

USING THE RELATIONSHIP FOR R_0,

$$\left.\frac{\partial^2 U}{\partial R^2}\right|_{R_0} = N\left(\frac{(n+1)\, 2\ln 2\; q^2}{R_0^3} - \frac{2(2\ln 2)q^2}{R_0^3}\right)$$

SO THAT PER UNIT LENGTH,

$$\frac{\left.\frac{\partial^2 U}{\partial R^2}\right|_{R_0}}{2NR_0} = \frac{2\ln 2\, q^2 (n-1)}{2R_0^4}$$

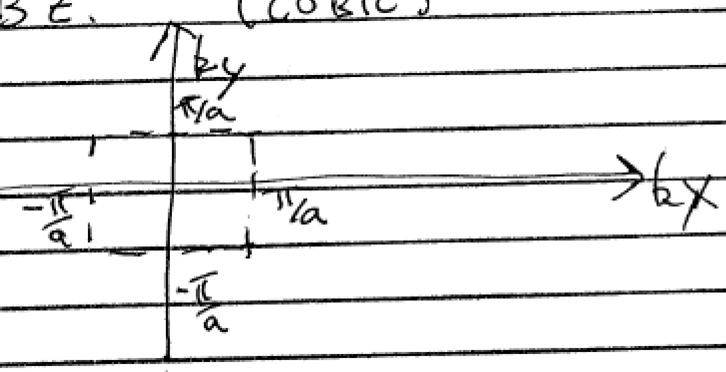
AND $C = R_0^2 \left.\frac{\partial^2 U}{\partial R^2}\right|_{R_0} =$

$$\boxed{C = \frac{(n-1)\ln 2\; q^2}{R_0^2}}$$

Chapter 7.

1.

(A) BZ: (CUBIC)



IN CORNER, $\vec{k} = (\pm\pi/a, \pm\pi/a) = (k_x, k_y)$

SO $\varepsilon_{CORNER} = \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar^2 \pi^2\, 2}{2m^* a^2}$

IN MIDDLE $\vec{k} = (k_x, k_y) = \left(\pm\frac{\pi}{a}, 0\right)$

OR $\left(0, \pm\frac{\pi}{a}\right)$

SO

$$\mathcal{E}_{MIDDLE} = \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar^2 \pi^2}{2m^* a^2} 1$$

SO $\boxed{\mathcal{E}_{CORNER} = 2\,\mathcal{E}_{MIDDLE}}$

(B) FOR 3D CUBIC

$$\vec{k}_{CORNER} = \left(\pm\frac{\pi}{a}, \pm\pi/a, \pm\frac{\pi}{a}\right) \quad (ETC)$$

SO $\mathcal{E}_{CORNER} = \frac{\hbar^2 \pi^2}{2m^* a^2} 3$

$$\vec{k}_{MIDDLE} = (k_x, k_y, k_z) = \left(\pm\frac{\pi}{a}, \pm\frac{\pi}{a}, 0\right)$$

(ETC. FOR PERMUTATIONS)

SO

$$\mathcal{E}_{MIDDLE} = \frac{\hbar^2 \pi^2}{2m^* a} 2$$

AND $\boxed{\mathcal{E}_{CORNER} = \frac{3}{2}\,\mathcal{E}_{MIDDLE}}$

(SOME PEOPLE DID THE MIDDLE OF THE "FACE" NOT "EDGE")

$$\vec{k}_{\substack{FACE \\ (MIDDLE)}} = \left(\pm\frac{\pi}{a}, 0, 0\right) \text{ ETC.}$$

SO $\boxed{\mathcal{E}_{CORNER} = 3\,\mathcal{E}_{FACE}}$

(E) FOR DIVALENT METAL,

2 e^- PER UNIT CELL. $\Rightarrow$

$$\text{DENSITY} = n = \frac{2}{a^3}$$

HENCE, $k_f = \left(3\pi^2 n\right)^{1/3}$

$$k_f = \frac{\left(6\pi^2\right)^{1/3}}{a} = \left(\frac{6}{\pi}\right)^{1/3}\left(\frac{\pi}{a}\right)$$

$k_f \approx 1.24\left(\pi/a\right)$

SO $k_f > k_{\substack{MIDDLE \\ FACE}} \Rightarrow$ FERMI SURFACE

GOES THROUGH MIDDLE FACE

HENCE 2 BANDS ARE PARTIALLY FULL $\Rightarrow$ METAL.