Assignment 2

1) Zero point kinetic energy $= \frac{(h/\lambda)^2}{2m}$

$\simeq \frac{h^2}{8mL^2}$ since $\lambda \sim 2L$.

$\sim \frac{(6.64\times10^{-27}\ \text{erg sec})^2}{8\times4\times1.67\times10^{-24}\times(10^{-8})^2}$

$\sim 8\times10^{-15}$ erg.

$\sim 5\times10^{-3}$ eV.

2) From notes:

$$U = 2N\epsilon\left\{\left(\frac{\epsilon}{r}\right)^{12}\sum_j p_{ij}^{-12} - \left(\frac{\epsilon}{r}\right)^{6}\sum_j p_{ij}^{-6}\right\}$$

By minimizing U w.r.t. $r \Rightarrow \frac{r}{\sigma} = 1.09$.

$$\therefore U = 2N\epsilon\left\{\left(\frac{1}{1.09}\right)^{12}\underbrace{\sum_j p_{ij}^{-12}}_{H} - \left(\frac{1}{1.09}\right)^{6}\underbrace{\sum_j p_{ij}^{-6}}_{I}\right\}$$

For F.C.C. $H = 12.13$ $I = 14.45$

B.C.C. $H = 9.11$ $I = 12.25$

$$\Rightarrow \frac{U_{B.C.C.}}{U_{F.C.C.}} = .956$$

3) From previous problem:

$U_{FCC} = 2.15 \times 4 N\epsilon$ for N atoms in crystal

$\therefore$ cohesive energy / mole $= 2.15 \times 4 \times 6 \times 10^{23} \times 50 \times 10^{-16}$ erg

$= 2.58$ kJ / mole.