Homework 3 Solutions

2. bcc: $U(R) = 2N\varepsilon[9.114(\sigma/R)^{12} - 12.253(\sigma/R)^6]$. At equilibrium $R_0^{\,6} = 1.488\sigma^6$, and $U(R_0) = 2N\varepsilon(-2.816)$.

fcc: $U(R) = 2N\varepsilon[12.132(\sigma/R)^{12} - 14.454(\sigma/R)^6]$. At equilibrium $R_0^{\,6} = 1.679\sigma^6$, and $U(R_0) = 2N\varepsilon(-4.305)$. Thus the cohesive energy ratio bcc/fcc = **0.956**, so that the fcc structure is more stable than the bcc.

3.
$$\begin{aligned} |U| &= 8.60\ N\varepsilon \\ &= (8.60)(6.02\times10^{23})\ (50\times10^{-16}) = 25.9\times10^{9}\ \text{erg/mol} \\ &= 2.59\ \text{kJ/mol}. \end{aligned}$$

This will be decreased significantly by quantum corrections, so that it is quite reasonable to find the same melting points for H_2 and Ne.

5a.

$$U(R) = N\left(\frac{A}{R^n} - \frac{\alpha q^2}{R}\right)\ ;\ \ \alpha = 2\ \log 2 = \text{ Madelung const.}$$

In equilibrium

$$\frac{\partial U}{\partial R} = N\left(-\frac{nA}{R_0^{n+1}} + \frac{\alpha q^2}{R_0^{\,2}}\right) = 0\ ;\ \ R_0^{\,n} = \frac{nA}{\alpha q^2},$$

and

$$U(R_0) = -\frac{N\alpha q^2}{R_0}(1 - \frac{1}{n}).$$

b. $$U(R_0\text{-}R_0\delta) = U(R_0) + \frac{1}{2}\frac{\partial^2 U}{\partial R^2}R_0(R_0\delta)^2 + \ldots,$$

bearing in mind that in equilibrium $(\partial U/\partial R)_{R_0} = 0.$

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

For a unit length $2NR_0 = 1$, whence

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

8. From (37) we have $e_{XX} = S_{11}X_X$, because all other stress components are zero. By (51), $3S_{11} = 2/(C_{11} - C_{12}) + 1/(C_{11} + C_{12})$.

Thus $Y = (C_{11}{}^2 + C_{12}C_{11} - 2C_{12}{}^2)/(C_{11} + C_{12})$;

further, also from (37), $e_{yy} = S_{21}X_x$,

whence $\sigma = e_{yy}/e_{xx} = S_{21}/S_{11} = -C_{12}/(C_{11} + C_{12})$.