LENNARD - JONES : SUMMARY

$$U_{total} = 2N\varepsilon\left[A_{12}\left(\frac{\sigma}{R_1}\right)^{12} - A_6\left(\frac{\sigma}{R_1}\right)^{6}\right] \quad ; \quad \frac{R_1(eq)}{\sigma} = \left(\frac{2A_{12}}{A_6}\right)^{1/6}$$

N = # Atoms

R_1 = Nearest Neighbour distance

$$A_n = \sum_j N_j \, \alpha_j^{-n}$$

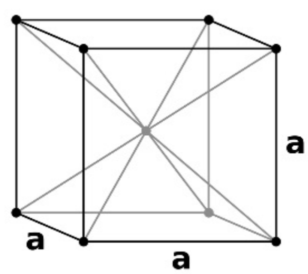
Where

N_j = j-order # neighbour atoms

$\alpha_j = R_j / R$

R_j = j-order neighbour distance

BCC $\quad \frac{R_1}{\sigma} = 1.07$



$N_1 = 8 \quad R_1 = \frac{\sqrt{3}}{2}a \quad \alpha_1 = 1$

$N_2 = 6 \quad R_2 = a \quad \alpha_2 = \frac{2}{\sqrt{3}}$

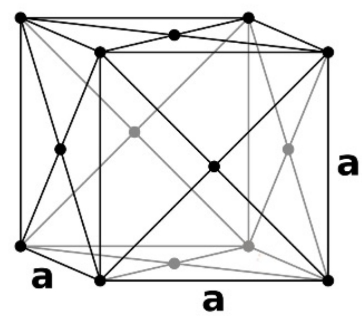
$N_3 = 12 \quad R_3 = \sqrt{2}\,a \quad \alpha_3 = 2\sqrt{\frac{2}{3}}$

$$A_6 = 8 \cdot \frac{1}{1^6} + 6 \cdot \frac{1}{(2/\sqrt{3})^6} + 12\frac{1}{\left(2\cdot\sqrt{\frac{2}{3}}\right)^6} + \ldots = 12.25$$

$$A_{12} = 8\frac{1}{1^{12}} + 6\frac{1}{(2/\sqrt{3})^{12}} + 12\frac{1}{\left(2\sqrt{\frac{2}{3}}\right)^{12}} + \ldots = 9.11$$

$$U_{total} = 2N\varepsilon(-4.03)$$

FCC $\quad \frac{R_1}{\sigma} = 1.09$



$N_1 = 12 \quad R_1 = \frac{\sqrt{2}}{2}a \quad \alpha_1 = 1$

$N_2 = 6 \quad R_2 = a \quad \alpha_2 = \frac{2}{\sqrt{2}}$

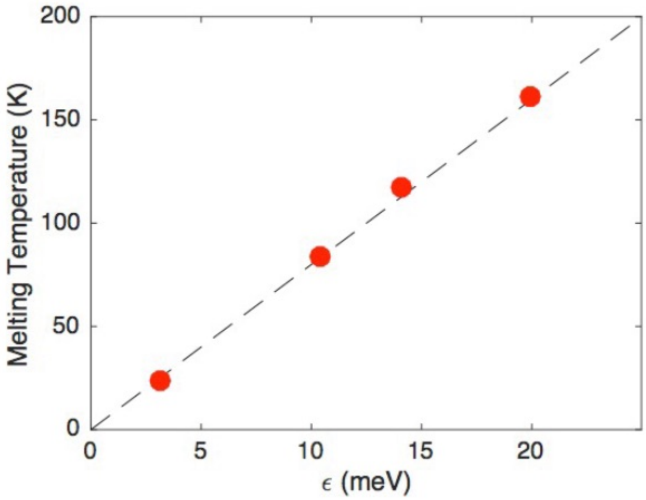
$N_3 = 24 \quad R_3 = \sqrt{\frac{3}{2}}\,a \quad \alpha_3 = \sqrt{3}$

$$A_6 = 12 + 6 \cdot \left(\frac{2}{\sqrt{2}}\right)^{-6} + 24 \cdot (\sqrt{3})^{-6} + \ldots = 14.45$$

$$A_{12} = 12 + 6\left(\frac{2}{\sqrt{2}}\right)^{-12} + 24(\sqrt{3})^{-12} + \ldots = 12.13$$

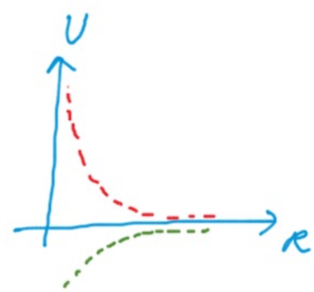
$$U_{total} = 2N\varepsilon(-4.3)$$

Melting temperature



Ionic Bonds:

$$U_{ij} = \begin{cases} \lambda \cdot \exp\left(\frac{-R}{\rho}\right) - \frac{q^2}{4\pi\varepsilon_0 R} & (NN) \\ \pm \frac{q^2}{4\pi\varepsilon_0 R} \frac{1}{p_{ij}} & \end{cases}$$



$\cdots \ominus \quad \oplus \quad \ominus \quad \oplus \quad \ominus \cdots$

2N atoms

$$U_{total} = N \cdot \sum_{ij} U_{ij}$$

$$= N \cdot \left(\#NN \cdot \lambda \cdot \exp\left(\frac{-R}{\rho}\right) - \frac{\alpha q^2}{4\pi\varepsilon_0 R} \right)$$

where $\alpha = \sum_j \frac{\pm}{p_{ij}} \equiv$ Madelung's constant

Ionic Bonds: CONTINUED

$$\frac{d\,U_{total}}{d\,R} = 0 \Rightarrow N\left\{ -\frac{[\#NN]\,\lambda}{\rho}\exp\left(-\frac{R}{\rho}\right) + \frac{\alpha q^2}{4\pi\varepsilon_0 R^2}\right\} = 0$$

$$\Rightarrow R_0^2 \cdot \exp\left(-\frac{R_0}{\rho}\right) = \frac{\alpha q^2 \cdot \rho}{4\pi\varepsilon_0}\,\frac{1}{\lambda\,[\#NN]}$$

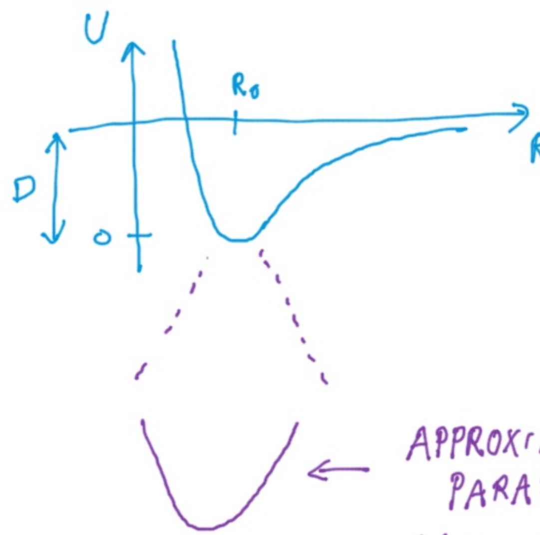
$$U_{total}(R_0) = N\left[\#NN \cdot \lambda \cdot \exp\left(\frac{-R_0}{\rho}\right) - \frac{\alpha q^2}{4\pi\varepsilon_0 R_0}\right]$$

$$= N \cdot \left[\frac{\alpha q^2 \rho}{4\pi\varepsilon_0 R_0^2} - \frac{\alpha q^2}{4\pi\varepsilon_0 R_0}\right]$$

$$= \frac{-N\alpha q^2}{4\pi\varepsilon_0 R}\left[1 - \frac{\rho}{R_0}\right]$$

MORSE POTENTIAL:

$$U = D \cdot \left\{1 - \exp\left(-a\,(R - R_0)\right)\right\}^2$$



APPROXIMATELY PARABOLIC

$U \propto (R - R_0)^2$

$\delta \equiv R - R_0$

= distance to equilibrium R_0