Determination of range of repulsive interaction

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Determination of range of repulsive interaction $\rho = ?$

$$B \text{ (Bulk modulus)} = \frac{\text{stress}}{\text{strain}}$$

$$B = \frac{F/A}{\Delta V/V} = \frac{dP}{dV} \times V$$

$$B = \frac{dP}{dV} \times V \quad \text{— (i)}$$

1st law of thermodynamics

$$dQ = dU + dW$$

take work-done on the system -ve by applying pressure dP so

$$dQ = dU - dW$$

For adiabatic compression by applying pressure dp $\quad dQ = 0$

$$0 = dU - PdV \qquad \because W = Pdv$$

$$dU = PdV$$

$$\frac{dU}{dv} = P$$

$$P = \frac{dU}{dV}$$

derivative w.r.t volume V

$$\frac{dP}{dV} = \frac{d^2U}{dV^2}$$

put in eq (i)

$$B = \frac{d^2U}{dV^2} \times V \quad \text{— (ii)}$$

using chain rule of derivative

$$\frac{dU}{dV} = \frac{dU}{dR} \times \frac{dR}{dV} \quad \text{— (iii)}$$

diffrentiate on both sides w.r.t 'V'

$$\frac{d}{dV}\left(\frac{dU}{dV}\right) = \frac{dU}{dR} \cdot \frac{d^2R}{dV^2} + \frac{dR}{dV} \cdot \left[\frac{d}{dV}\left(\frac{dU}{dR}\right)\right]$$

$$\frac{d^2U}{dV^2} = \frac{dU}{dR} \cdot \frac{d^2R}{dV^2} + \frac{dR}{dV} \cdot \left[\frac{d}{dV}\left(\frac{dU}{dR}\right)\right]$$

$$= \frac{dU}{dR} \cdot \frac{d^2R}{dV^2} + \frac{dR}{dV}\left[\frac{d}{dR}\left(\frac{dU}{dV}\right)\right]$$

put value of $\frac{dU}{dV}$ from eq (iii)

$$\frac{d^2U}{dV^2} = \frac{dU}{dR}\cdot\frac{d^2R}{dV^2} + \frac{dR}{dV}\left[\frac{d}{dR}\underbrace{\left(\frac{dU}{dR} \times \frac{dR}{dV}\right)}\right]$$

apply product rulue of derivative

$$\frac{d^2U}{dV^2} = \frac{dU}{dR}\cdot\frac{d^2R}{dV^2} + \frac{dR}{dV}\left[\frac{d^2U}{dR^2} \times \frac{dR}{dV} + \frac{dU}{dR} \times \frac{d}{dR}\left(\frac{dR}{dV}\right)\right]$$

Now at $R = R_0$

$$\frac{dU}{dR} = 0$$

$$\frac{d^2U}{dV^2} = 0 + \frac{dR_0}{dV}\left[\frac{d^2U}{dR_0^2} \times \frac{dR_0}{dV} + 0\right]$$

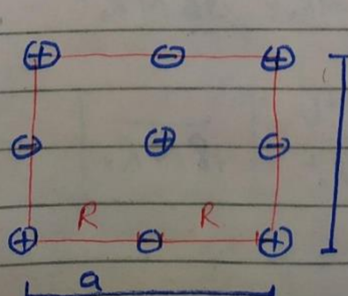
$$\frac{d^2U}{dV^2} = \frac{d^2U}{dR_0^2} \times \left(\frac{dR_0}{dV}\right)^2$$

$\because \frac{dR}{dV} \times \frac{dR}{dV} = \left(\frac{dR}{dV}\right)^2$

put this value of $\frac{d^2U}{dV^2}$ in eq (ii)

$$B = \frac{d^2U}{dR_0^2}\left(\frac{dR_0}{dV}\right)^2 \times V \quad \text{— (iv)}$$

for NaCl crystall (fcc structure)



$a = 2R$

$a^3 = 8R^3$

$V = 8R^3$

4 atoms per unit cell in fcc

$$V = \frac{8R^3}{4} = 2R^3$$

there are N atoms

$$V = 2NR^3$$

$$\frac{dV}{dR} = 2N(3R^2)$$

$$\frac{dV}{dR} = 6NR^2$$

inverse both sides

$$\frac{dR}{dV} = \frac{1}{6NR^2}$$

put in eq (iv)

V

$$B = \frac{d^2U}{dR_0^2}\left(\frac{1}{6NR_0^2}\right)^2 (2NR_0^3)$$

$$= \frac{d^2U}{dR_0^2}\,\frac{1}{36N^2R_0^4}\,(2NR_0^3)$$

$$B = \frac{d^2U}{dR_0^2}\left[\frac{1}{18NR_0}\right] \quad \text{— (v)}$$

we know that

$$\frac{dU}{dR} = \frac{-NZ\lambda}{\rho} e^{-R/\rho} + \frac{N\alpha q^2}{R^2} \quad \text{— (A)}$$

$R = R_0 \qquad \frac{dU}{dR} = 0$

$$0 = \frac{-NZ\lambda}{\rho} e^{-R_0/\rho} + \frac{N\alpha q^2}{R_0^2}$$

$$\frac{\cancel{N}Z\lambda}{\rho} e^{-R_0/\rho} = \frac{\cancel{N}\alpha q^2}{R_0^2}$$

$$e^{-R_0/\rho} = \frac{\rho\alpha q^2}{Z\lambda R_0^2}$$

diff eq A w.r.t R

$$\frac{d^2U}{dR_0^2} = \frac{\cancel{N}Z\lambda}{\rho^2} e^{-R_0/\rho} - \frac{2N\alpha q^2}{R_0^3}$$

$$= \left[\frac{NZ\lambda}{\rho^2}\left(\frac{\rho\alpha q^2}{Z\lambda R_0^2}\right) - \frac{2N\alpha q^2}{R_0^3} \right]$$

$$\frac{d^2U}{dR_0^2} = \frac{\alpha q^2}{R_0^2}\left[\frac{R_0}{\rho} - 2\right]$$

put in eq (v)

$$B = \frac{\alpha q^2}{18 R_0^4}\left[R_0/\rho - 2\right]$$