Bulk Modulus (Elastic Modulus)

$F = -kx$

$$K = B = \frac{\text{stress}}{\text{strain}} = -V\frac{\partial P}{\partial V}$$

← pressure

↑ volume

$$= \frac{-dP\ (\text{stress})}{\left(\frac{dV}{V}\right)\ (\text{strain})}$$

– some texts

Thermodynamics: $TdS = dU + PdV$

$T \sim 0K$

$$P = -\frac{\partial U}{\partial V} \Rightarrow -\frac{\partial P}{\partial V} = \frac{\partial^2 U}{\partial V^2} \Rightarrow B = V\frac{\partial^2 U}{\partial V^2}$$

$$\frac{\partial U}{\partial V} = \frac{\partial U}{\partial R}\frac{\partial R}{\partial V}$$

$$\left.\frac{\partial^2 U}{\partial V^2}\right|_{R=R_0} = \left[\frac{\partial^2 U}{\partial R^2}\left(\frac{\partial R}{\partial V}\right)^2 + \frac{\partial U}{\partial R}\frac{\partial^2 R}{\partial V^2}\right]_{R=R_0}$$

$\frac{\partial U}{\partial R} \to 0$ when $R = R_0$

Ionic crystal

$$U(R) = N\left(z\lambda e^{-\frac{R}{\rho}} - \frac{\alpha q^2}{R}\right)$$ cgs

$$\frac{dU}{dR} = N\left(-\frac{z\lambda}{\rho}e^{-R/\rho} + \frac{\alpha q^2}{R^2}\right)$$

$$\frac{d^2U}{dR^2} = N\left(\frac{z\lambda}{\rho^2}e^{-R/\rho} - \frac{2\alpha q^2}{R^3}\right)$$

$$\left.\frac{d^2U}{dR^2}\right|_{R=R_0} = N\left(\frac{z\lambda}{\rho^2}e^{-\frac{R_0}{\rho}} - \frac{2\alpha q^2}{R_0^3}\right)$$

$$\frac{\rho\alpha q^2}{z\lambda R_0^2}$$

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

$$= N\frac{\alpha q^2}{R_0^3}\left(\frac{R_0}{\rho} - 2\right)$$

$$V = \frac{Na^3}{4} \qquad a = 2R \longrightarrow V = 2NR^3$$

fcc

$$\frac{\partial V}{\partial R} = 6NR^2 \Rightarrow \left(\frac{\partial R}{\partial V}\right)^2 = \frac{1}{36N^2R^4}$$

$$B\Big|_{R_0} = V\left.\frac{\partial^2 U}{\partial V^2}\right|_{R_0} = V\left.\frac{\partial^2 U}{\partial R^2}\left(\frac{\partial R}{\partial V}\right)^2\right|_{R_0}$$

$$= (2\pi R_0^3)\left[\frac{N\alpha q^2}{R_0^3}\left(\frac{R_0}{s}-2\right)\right]\left(\frac{1}{36\pi^2 R_0^4}\right)$$

$$= \frac{\alpha q^2}{18 R_0^4}\left(\frac{R_0}{s}-2\right)$$

$Zn\,S$ diamond

ionic or covalent $Zn^{++}\,S^{--}$