We seek relationship between the following parameters:

(i) E Young's Modulus GPa

(ii) Ω volume per atom or molecule (e.g. Cu or ZrO_2) $= \frac{M_W}{\rho N_A}$ $\boxed{\begin{array}{l} a = \Omega^{1/3} \\ A = \Omega^{2/3} \end{array}}$

(iii) ΔH_v enthalpy of formation (it may be the heat of melting or the heat of vaporization) ✓ Since the modulus goes to zero when the crystal melts,

(iv) Z - coordination number

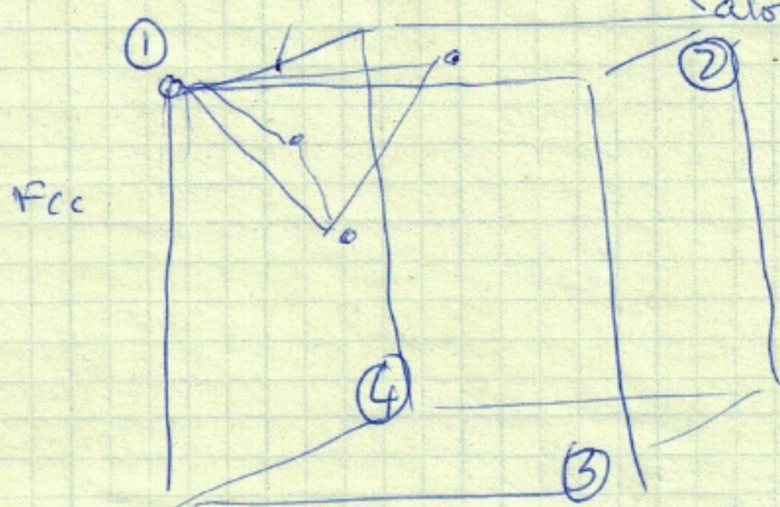
Simple Cubic 6

FCC 12

BCC 8

Hexagonal 12

Structure of Diamond



sp^3

$\boxed{\begin{array}{c} \text{8 atoms per unit cell} \\ Z = 4 \end{array}}$

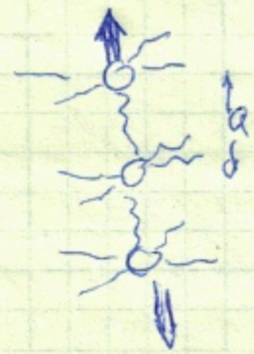
8 tetrahedra - one from each corner but only 4 are occupied

$8 = 4\,(fcc) + 4\,(\text{tetrahedra})$

Bond stretch-stiffness model

Step 1

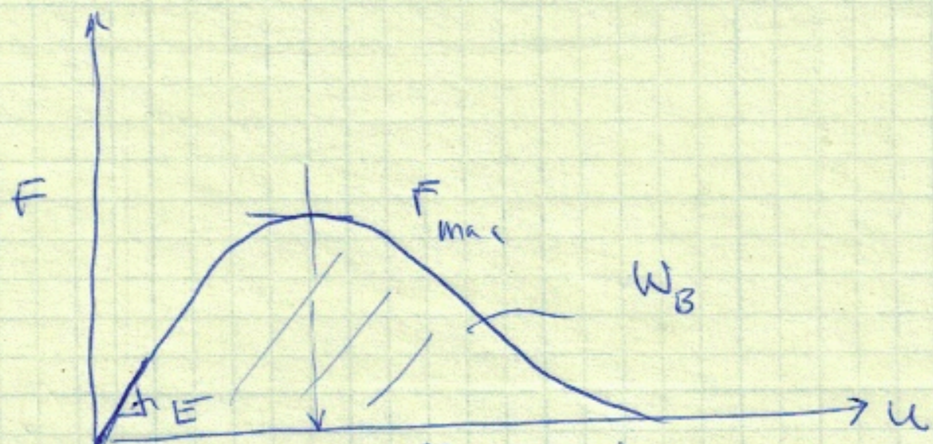
assume a simple cubic structure



Step 2

Draw an approximate Force/displacement curve
F, u

$$\sigma = \frac{F}{\Omega^{2/3}} \qquad \epsilon = \frac{u}{a} \quad \text{(uniaxial tension)}$$

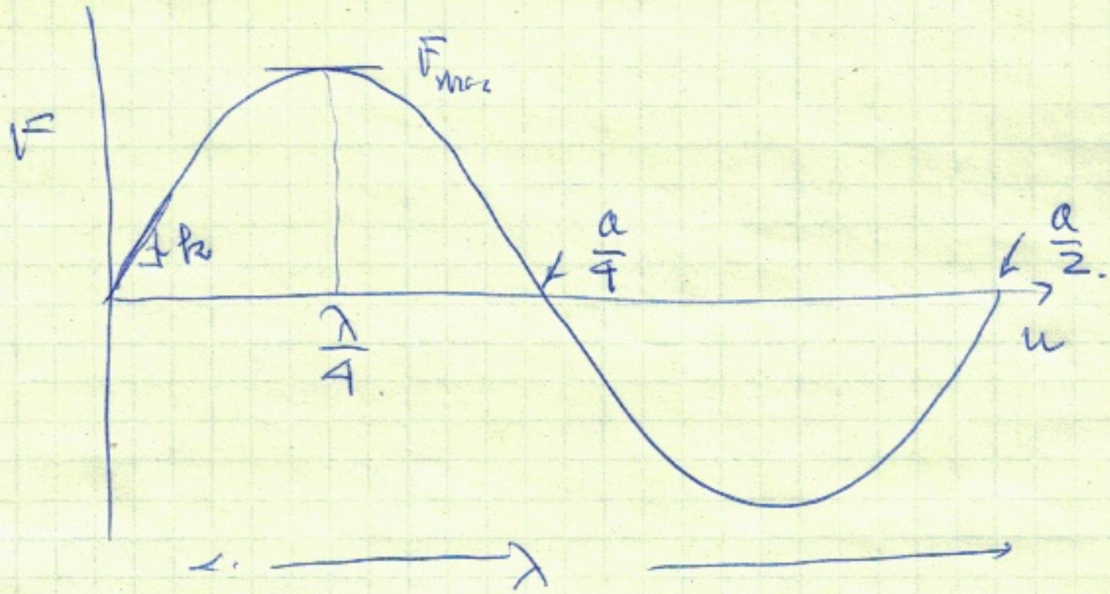


$$\epsilon_S = \frac{u(F_{max})}{a} \approx 12.5\% = \frac{1}{8}$$

in reality 10% - 15%.

Step 3 Formal shape of the (F, u) curve.

$$F = F_{max} \sin \frac{2\pi u}{\lambda}$$



$$u(F_{max}) = \frac{\lambda}{4} = \frac{a}{8}$$

$$\boxed{\therefore \lambda = \frac{a}{2}} = \frac{\Omega^{1/3}}{2} \quad \text{— (1)}$$

$$F = F_{max} \sin \frac{2\pi u}{\lambda}.$$

Stiffness & modulus

$$k = \frac{\Delta F}{\Delta u} = \frac{\Delta\sigma \times \Omega^{2/3}}{\Delta\epsilon\, \Omega^{1/3}}$$

$$= E\,\Omega^{1/3}$$

$$E = \frac{k}{\Omega^{1/3}} \quad \text{— (2)}$$

Wb

$$k = \left|\frac{dF}{du}\right|_{u\to 0} = \frac{2\pi F_{max}}{\lambda}\left(\cos\frac{2\pi u}{\lambda}\right)_{u\to 0 \atop \to 1}$$

$$k = \frac{2\pi F_{max}}{\lambda}$$

$$\boxed{k = \frac{4\pi F_{max}}{\Omega^{1/3}}} \quad \text{— (3)}$$

$$\lambda = \frac{\Omega^{1/3}}{2}$$

$\underline{W_B}$ work for bond.

$$W_B = \int_0^{\lambda/2} F_{max} \sin \frac{2\pi u}{\lambda}\, du$$

$$= F_{max} \frac{\lambda}{2\pi} \underbrace{\left[-\cos \frac{2\pi u}{\lambda} \right]_0^{\lambda/2}}_{=2}$$

$$= \frac{F_{max} \lambda}{\pi} = F_{max} \frac{\Omega^{1/3}}{2\pi}$$

$$\boxed{W_B = \frac{F_{max}\, \Omega^{1/3}}{2\pi}} \quad \text{— (4)}$$

(2) + (3) (3) + (4)

$$W_B = \frac{\Omega^{1/3}}{2\pi} \times \frac{\Omega^{1/3} k}{4\pi}$$

$$k = E\Omega^{1/3}$$

$$\Rightarrow W_B = \frac{E\Omega}{8\pi^2}.$$ related to packing

aside

$$\Omega = \frac{M_w}{\rho N_A}$$

$$= \frac{E}{\rho} \times \frac{M_w}{N_A} \times \frac{1}{8\pi^2}.$$ (SC)

$\Delta H_V \leftrightarrow W_B$

Extend simple cubic or other structures with higher coordination

$$Z \to Z^*$$

$$W_B \to W_B^* \to \Delta H_V = W_B^* \frac{Z}{2} \text{ (per atom).}$$

$$E \to E^*$$

$$E^* = E \times \frac{Z}{6}$$

$$W_B^* \text{ (all bonds)} = \cancel{\frac{\Omega}{8\pi^2}} \cdot \frac{E^* 6}{\cancel{Z}} \times \frac{\cancel{Z}}{2}$$

(2) shared between two atoms.

$$W_B^* = \frac{6E^*}{Z} \times \frac{\Omega}{8\pi^2}$$

$$\Delta H_V = \frac{\cancel{Z}}{\cancel{2}} \cdot \frac{\overset{3}{\cancel{6}}E^*}{\cancel{Z}} \times \frac{\Omega}{8\pi^2}$$

$$\boxed{E^* = \frac{8\pi^2}{3\Omega} \cdot \Delta H_V}$$

heat of melting