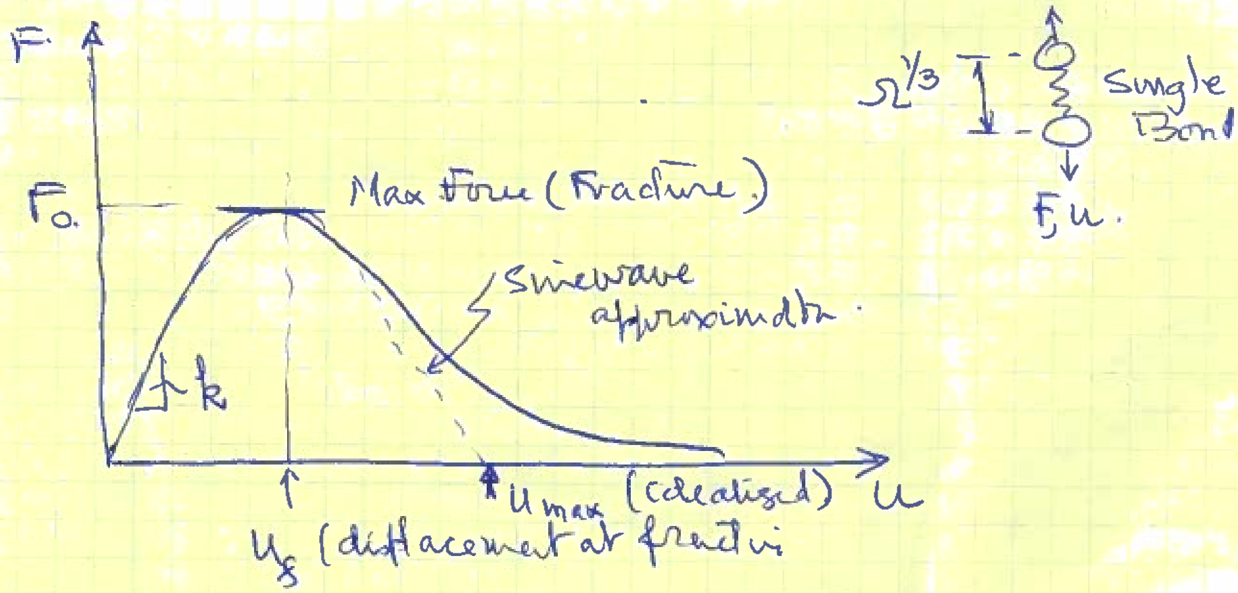
Derivation for The Relationship Between the Heat of Evaporation ($\Delta H_v$; J/mol) and the Young's Modulus ($E$, Pa) and its application to Copper.




Features of the curve:

(i) Initial slope corresponds to the spring constant

$$k = \left(\frac{dF}{du}\right)_{u \to 0}$$

(ii) Fracture occurs the $F = F_0$ & $u = u_f$.

tensile strain at fracture

$$\epsilon_f = \frac{u_f}{\Omega^{1/3}}$$

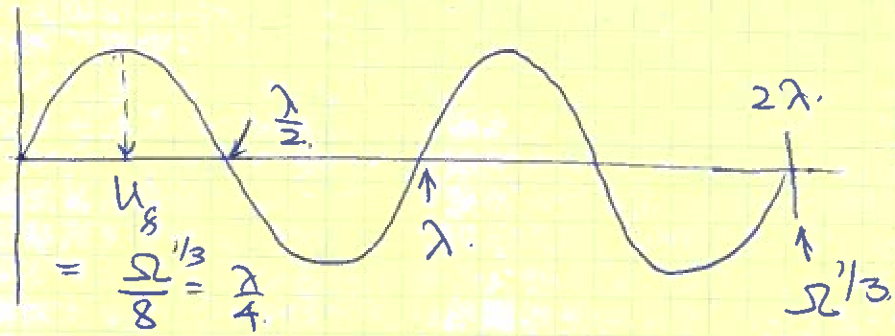
(iii) Area under the curve. i.e. $\displaystyle\int_0^{u_{max}} F\,du$

is equal to the work done to break the bond. It is the "energy" of the bond $= W_B$

(IV). <u>Assumptions</u>:

(a) Approximate the curve by a half sine-wave of wave length $\lambda$.

(b) $$F = F_0 \sin \frac{2\pi u}{\lambda} \quad \text{———} ①$$




Since $\frac{u_g}{\Omega^{1/3}} = \epsilon_g = 12.5\%$ (from experiments with perfect specimens)

$$u_g = \frac{1}{8}\Omega^{1/3}$$

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

<u>Let us now calculate $W_B$</u>

$$W_B = \int_0^{\lambda/2} F_0 \sin \frac{2\pi u}{\lambda}\, du$$

$$= F_0 \frac{\lambda}{2\pi}\left[-\cos \frac{2\pi}{\lambda} u\right]_0^{\lambda/2}$$

$$= \left(F_0 \frac{\lambda}{2\pi}\right)(-1)\left(\underbrace{\cos \frac{\cancel{2}}{\cancel{2}}\pi}_{-1} - \underbrace{\cos(0)}_{1}\right)$$

$$W_B = F_0 \frac{\lambda}{2\pi} \times 2 = \frac{\lambda F_0}{\pi} \quad — (3)$$

Note units are energy (Joules) on both sides.

To obtain $F_0$ equate the initial slope = $k$. the spring constant.

$$\left(\frac{dF}{du}\right)_{u\to 0} = \frac{2\pi}{\lambda} \cdot F_0 \left[\cos \frac{2\pi u}{\lambda}\right]_{u\to 0} = k$$

$$k = \frac{2\pi}{\lambda} \times F_0 .$$

$$F_0 = \frac{\lambda k}{2\pi} \quad — (4)$$

(3) + (4) $\rightarrow$

$$\left.\begin{aligned} W_B &= \frac{\lambda}{\pi} \times \frac{\lambda k}{2\pi} \\ E &= \frac{k}{\Omega^{1/3}} \\ \lambda &= \frac{\Omega^{1/3}}{2} \end{aligned}\right\} \text{ combine}$$

$$W_B = \frac{\lambda^2}{2\pi^2} \times E\Omega^{1/3} = \frac{\Omega^{2/3}}{8\pi^2} \cdot E\Omega^{1/3} = \frac{E\Omega}{8\pi^2} \quad — (5)$$

Note units match since $E$ has units of energy per unit volume.

## Accounting for the coordination number Z

Z is the number of nearest neighbours

$$E_Z = \frac{Z}{6} E \qquad — (6)$$

$\uparrow$ modulus with correct NN

(5) + (6)

$$W_B = \frac{\Omega}{8\pi^2} \times \frac{6 E_Z}{Z} \qquad — (8)$$

## Relate $W_B$ to the Heat of Evaporation

$$\underset{\text{(per atom)}}{\Delta H_V} = W_B \left(\frac{\# \text{ Bonds}}{2}\right)$$

$\uparrow$ because one half of the bond energy is left behind.

$$= \frac{Z W_B}{2}$$

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

$$E_Z = \frac{\Delta H_V}{\Omega} \times \frac{8\pi^2}{3} \qquad — (*)$$

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Calaculate Omega for copper

| | | |
|---|---|---|
| At wt | 63.5 | g/mol |
| Density | 8.93 | g/cm^3 |
| Vol/mol | 7.11 | cm^3 |
| Avogadro | 6.03E+23 | atom/mol |
| Omega | 1.18E-23 | cm^3 |
| | 1.18E-29 | m^3 |
| Interatom spac | 2.28E-10 | m |
| Omega^(1/3) | 0.23 | nm |

COPPER (use heat of evaporation)
Calculation of the Elastic Modulus

$$\boxed{E_Z = \frac{8\pi^2}{3}\frac{\Delta H_V}{\Omega}}$$

| | | | | |
|---|---|---|---|---|
| Del_HV | 338 | kJ/mol | | |
| DeL_HV/atom | 5.61E-22 | kJ/atom | | |
| | 5.61E-19 | J/atom | DEL_H_V per atom | |
| Omega | 1.18E-29 | m^3 | | |
| E_z | 1.25E+12 | Pa | 1249 | GPa |

COPPER (use heat of melting)
Calculation of the Elastic Modulus

| | | | | |
|---|---|---|---|---|
| Del_H_fusion | 13.2 | kJ/mol | | |
| DeL_H_fus/atom | 2.19E-23 | kJ/atom | | |
| | 2.19E-20 | J/atom | | |
| Omega | 1.18E-29 | m^3 | | |
| E_z | 4.88E+10 | Pa | 49 | GPa |
| | | Experiment | 117 | GPa |