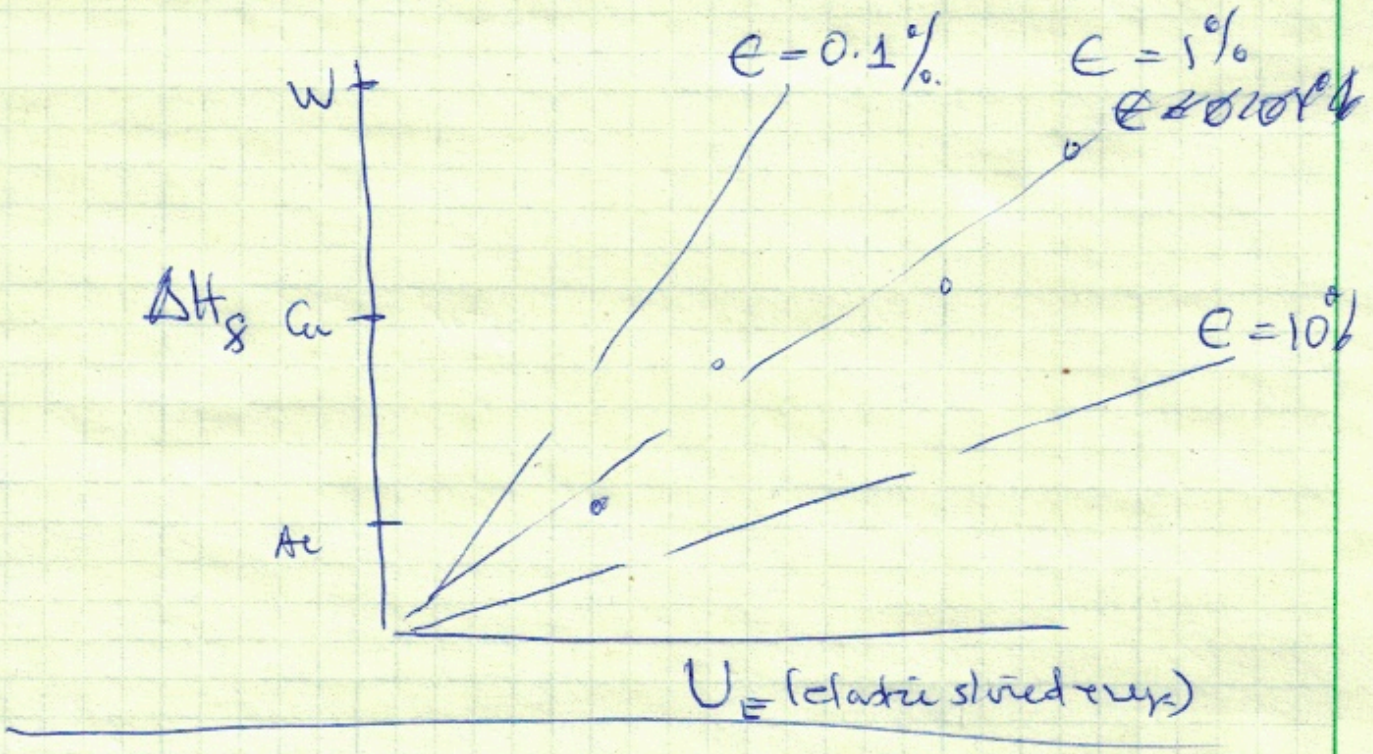
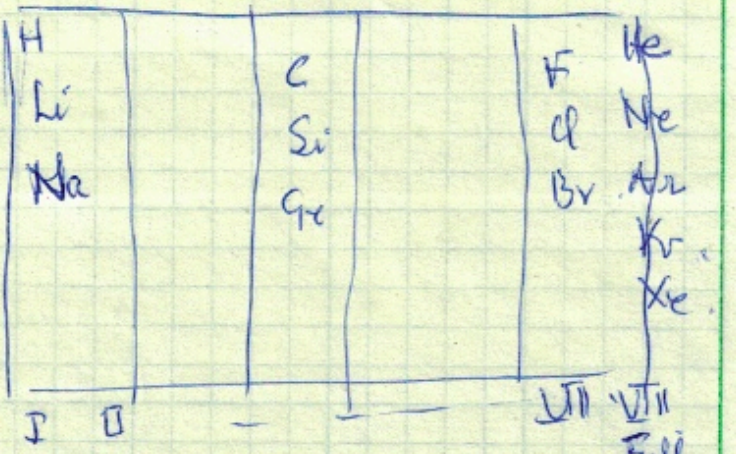
From previous lecture:



THE NATURE THE CHEMICAL BOND



THE PERIODIC TABLE

LEFT

"gives up electrons"

Shares Electrons

RIGHT

"wants electrons"

THE PERIODIC TABLE

s	2	spherical
p	6	Main Groups
d	10	directions.

Discrete s, p, d. 1s, 2s, 2p, 3s, 3p 3d.

Probabalistic The physical distribution of electrons around the nucleus is broad within a band.

~~Carbon~~

Metallic Al 3e

Covalent C 4e

Ionic NaCl. Na^+ e Cl^- (8) (8)

Metals → "free electrons" shared globally Weak

Covalent → shared locally. Strong

Ionic → transferred to create electrostatic bonds → Moderately strong

---

Metallic → "free" electrons that are shared globally.

Ionic/Covalent

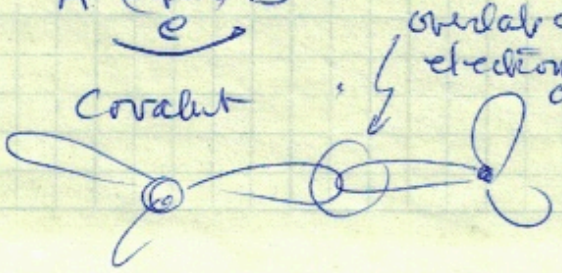
Often bonds are partially ionic/covalent

Ionic

A^+ dipole B^-

e

Covalent



BONDING - STRUCTURE

Isotropic bonds

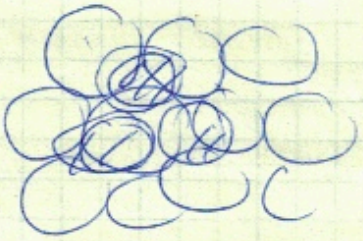
Ideal metallic

Ideal ~~covalent~~ ionic.

Maximize nearest neighbor # bonds per unit vol.

12 nearest neighbors.

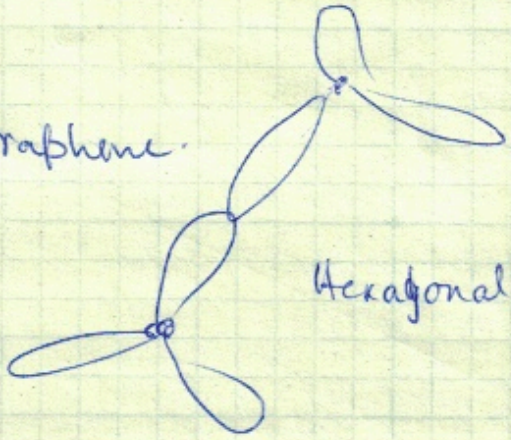
$Z = 12$



Fcc.

Highly Directional

graphene.



Hexagonal structure.

Often

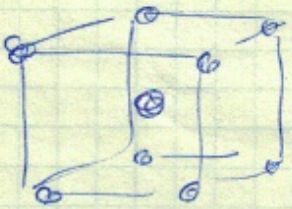
Bonds are mixed.

Metallic + covalent → Fe

B.C.C. structure.

8 NN

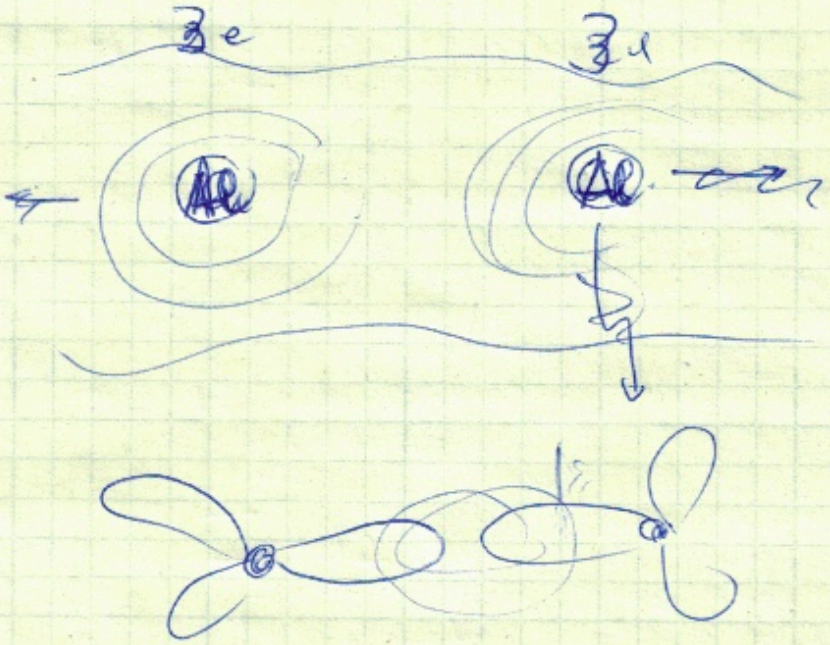
$Z = 8$

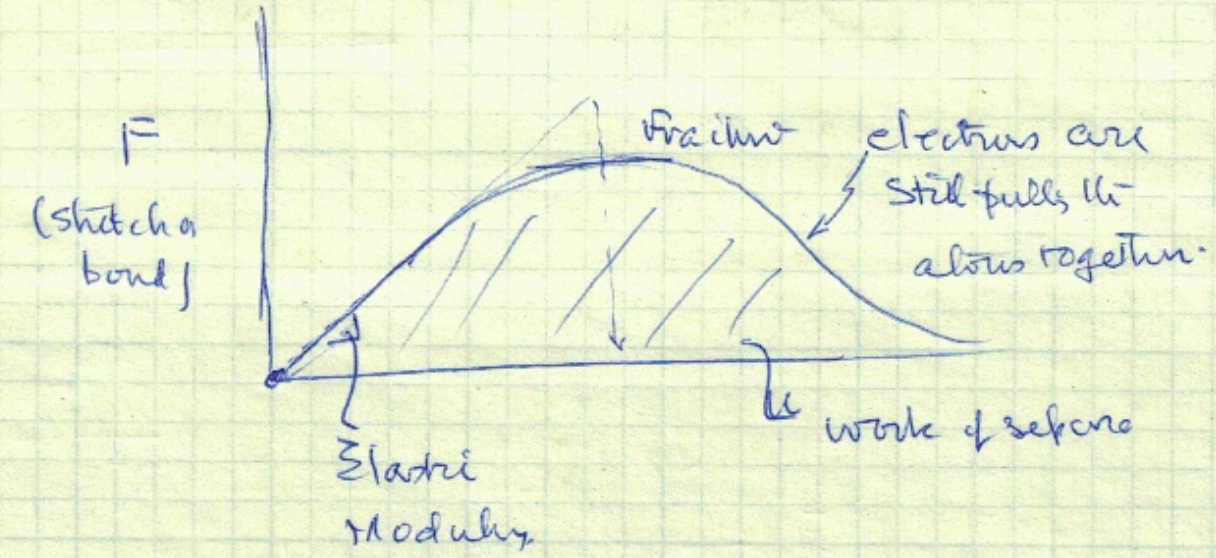


Ionic + covalent

electronegativity series

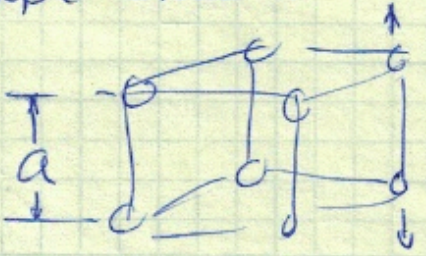
The world of electrons is probabilistic.





Model. Assume a simple structure

Simple cubic

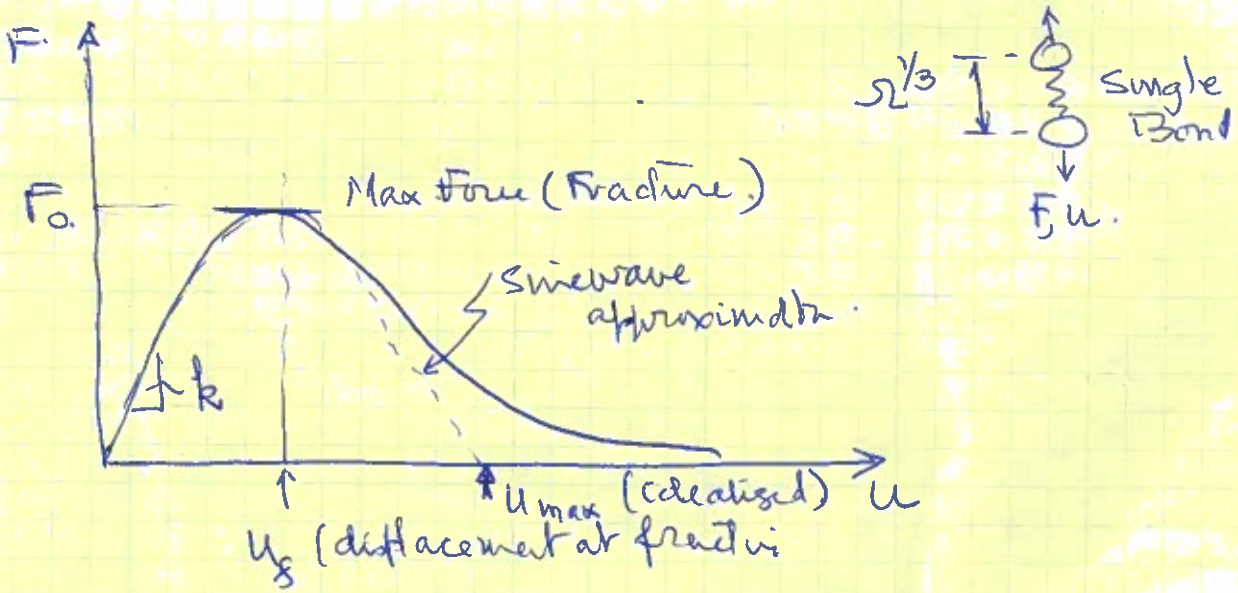


Structure parameters: $\Omega = a^3$.

a.

Z

Derivation for the Relationship Between the Heat of Evaporation (ΔH_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 $F = F_0$ & $u = u_s$.

tensile strain at fracture

$$\epsilon_s = \frac{u_s}{\Omega^{1/3}}$$

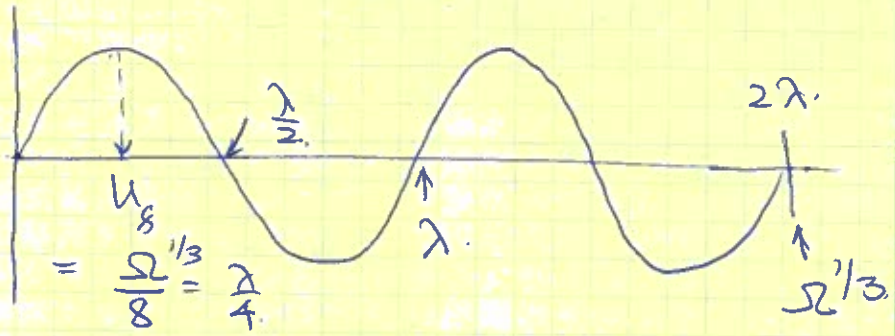
(iii) Area under the curve. i.e. $\int_0^{u_{max}} F\,du$

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

(IV). Assumptions:

(a) Approximate the curve by a half sine-wave of wave length λ.

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



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

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

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

Let us now calculate W_B

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

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

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

$-1 \quad -1$

$$W_B = \bar{F}_0 \frac{\lambda}{2\pi} \times 2 = \frac{\lambda \bar{F}_0}{\pi} \quad \text{— (3)}$$

Note units are energy (Joules) on both sides.

To obtain $\bar{F}_0$ equate the initial slope = k, the spring constant

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

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

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

(3) + (4) →

$$W_B = \frac{\lambda}{\pi} \times \frac{\lambda k}{2\pi}$$

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

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

} combine

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

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

$$E_Z = \frac{Z}{6}\bar{E} \qquad \text{— (6)}$$

↑ modulus with correct NN

(5) + (6)

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

Relate W_B to the Heat of Evaporation

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

↑ because one half of the bond energy is left behind.

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

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

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

Mech Prop Jan 24. 2018

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

Del_HV	338	kJ/mol
DeL_HV/atom	5.61E-22	kJ/atom
	5.61E-19	J/atom
Omega	1.18E-29	m^3

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

DEL_H_V per atom

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