Day-20

→ Surface energy (enthalpy)

Due to disarray of atoms and bonding patterns (causes an increase in entropy)

Excess +ve because the bonds form

- Broken bonds
- They are the lower energy state

Different bonding patterns associated with different planes → will have a different surface energy ($J\ m^{-2}$)

→ Surface energy of Cu:

Cu, CF lattice

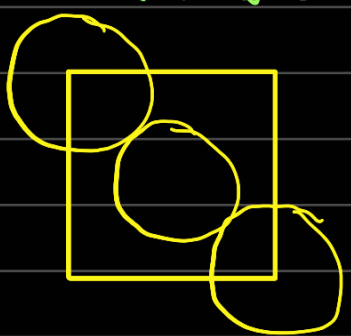
$r_{Cu} = 127.8\ \mu m$

Cu at (0,0,0)

Bond energy of Cu is $56.4\ kJ\ mol^{-1}$ of bonds

Calculate S.E. of (111) plane and compare with that of (110) and (100) planes

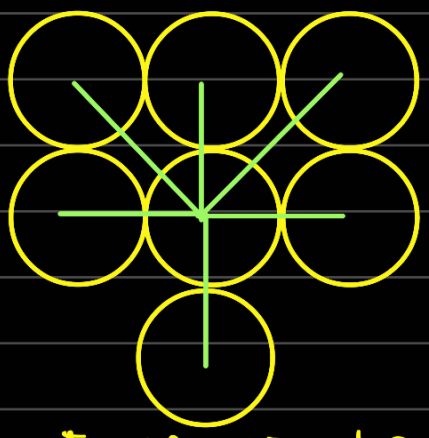
Ans.)



$4r = \sqrt{2}a$

$\Rightarrow a = 2\sqrt{2}r$

We have ABC stacking



6 bonds in plane
3 bonds go into plane of screen and 3 go out.

3 out of 12 bonds are broken

E_b = 56.4 kJ mol^{-1} of bonds
per Cu atom there are 12 bonds in this structure = $\frac{12}{N_A} \times \frac{E_b}{2} = \ell_b$

$$S.E. = \frac{3\ell_b}{12} \times P.D.$$

$$\frac{3\ell_b}{12} = \frac{3E_b}{2N_A}$$

$$P.D. \text{ of } (111) \text{ plane} = \frac{3\times 1/6 + 3\times 1/2}{\frac{\sqrt{3}}{4}(\sqrt{2}a)^2}$$

$$= \frac{2\times 4}{\sqrt{3}(4r)^2}$$

$$= \frac{8}{\sqrt{3}\times 16r^2}$$

$$= \frac{1}{2\sqrt{3}r^2}$$

$$\therefore S.E = \frac{3E_b}{2N_a} \times \frac{1}{2\sqrt{3}r^2}$$

$$= \frac{3\times 56.4\times 10^3}{2\times 6.022\times 10^{23}} \times \frac{1}{2\sqrt{3}\times (127.8\times 10^{-12})^2}$$

$= 2.483 \text{ J m}^{-2}$

→ Importance of grain boundary -

CdTe Solar cell
Na-lime glass → optical microscope

microstructure

Classified as Tilt or Twist boundary

General → combination of tilts + twists

Defect energy → GB energy
↓
Grain Boundary

☆ (From slides)

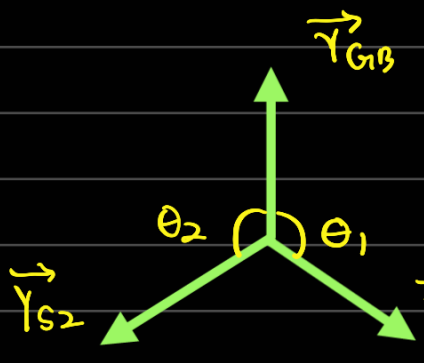
Let $S_1 : (h_1 k_1 l_1) \rightarrow \sigma_{h_1 k_1 l_1} \rightarrow \sigma_{S_1}$

$S_2 : (h_2 k_2 l_2) \rightarrow \sigma_{h_2 k_2 l_2} \rightarrow \sigma_{S_2}$

σ_S → S.E. of surface S
↓
Surface Energy

σ_{GB} (or γ_{GB})

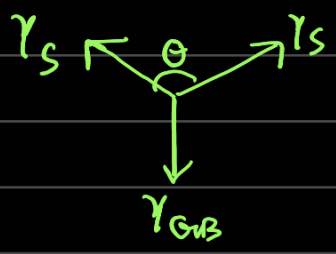
Equilibrium: $\vec{\gamma}_{S_1} + \vec{\gamma}_{S_2} + \vec{\gamma}_{GB} = 0$



$\gamma_{S_1} \cos\theta_1 + \gamma_{S_2} \cos\theta_2 = \gamma_{GB}$

$\gamma_{S_1} \sin\theta_1 = \gamma_{S_2} \sin\theta_2$

→



- GB bisects 2 surfaces
- $\theta = 161°$
- surface is {111} Cu.

Estimate γ_{GB}.

Ans) $\gamma_{GB} = 2\gamma_s \cos\theta/2$ ($\theta \rightarrow$ misorientation angle for this case)

$= 2\gamma_s \cos 80.5°$

$= 2 \times 2.483 \cos 80.5°$ J m^{-2}

$\simeq 0.82$ J m^{-2}