

## Solutions

☆ Vacancies in metals -

$$\begin{aligned} 1) \quad \frac{(n_v/N)_{T_1}}{(n_v/N)_{T_2}} &= \frac{e^{-\Delta H_v/RT_1}}{e^{-\Delta H_v/RT_2}} \\ &= e^{\frac{\Delta H_v}{R} \left( \frac{1}{T_2} - \frac{1}{T_1} \right)} \end{aligned}$$

$$\Rightarrow \Delta H_v = \frac{RT_1 T_2}{T_1 - T_2} \ln \left[ \frac{(n_v/N)_{T_1}}{(n_v/N)_{T_2}} \right]$$

$$\begin{aligned} \text{Take } T_1 &= 2410^\circ\text{C} = 2683\text{K} \\ T_2 &= 1234^\circ\text{C} = 1507\text{K} \end{aligned}$$

$$\begin{aligned} \therefore \Delta H_v &= \frac{8.314 \times 2683 \times 1507}{1176 \times 1000} \ln \left( \frac{5.26 \times 10^{-3}}{3.091 \times 10^{-5}} \right) \\ &\quad \text{kJ mol}^{-1} \\ &\approx 146.835 \text{ kJ mol}^{-1} \end{aligned}$$

$$= \frac{146835}{1.6 \times 10^{-19} \times 6.022 \times 10^{23}} \text{ eV/atom}$$

$$\approx \boxed{1.524 \text{ eV/atom}}$$

$$2) \quad \frac{(n_v/N)_{T_2}}{(n_v/N)_{T_1}} = e^{\frac{\Delta H_v}{R} \left( \frac{1}{T_1} - \frac{1}{T_2} \right)}$$

$$\begin{aligned} \Rightarrow \frac{1}{T_2} &= \frac{1}{T_1} - \frac{R}{\Delta H_v} \ln \left[ \frac{(n_v/N)_{T_2}}{(n_v/N)_{T_1}} \right] \\ &= \frac{1}{1161} - \frac{8.617}{1.5} \ln \left[ \frac{10^{-3}}{10^{-6}} \right] \end{aligned}$$

$$= \frac{1}{1161} - \frac{8.617}{1.5} \times 3 \ln 10 < 0$$

$$\Rightarrow T_2 < 0 \quad (\text{That's not possible!})$$

So it is not possible to achieve a vacancy fraction of one vacancy for every thousand atomic sites by simply raising the temperature.

$$3) \quad \frac{n_v}{N_A} = \frac{26.98}{26.2} \times \frac{7.57 \times 10^{23}}{10^6 \times 6.022 \times 10^{23}} \\ \approx 1.294 \times 10^{-6}$$

$$\text{Now, } 1.294 \times 10^{-6} = e^{\frac{-E_a}{RT}}$$

$$\Rightarrow E_a = -RT \ln(1.294 \times 10^{-6})$$

$$= \frac{8.617}{10^5} \times 873 \ln\left(\frac{10^6}{1.294}\right) \text{ eV/atom}$$

$$\approx \boxed{1.02 \text{ eV/atom}}$$

$$4) \quad n_v (\text{in m}^{-3}) = \exp\left(\frac{-1.08}{8.617 \times 10^{-5} \times 1123}\right) \times 6.022 \times 10^{23} \times \frac{7.65}{55.85} \\ \approx 1.173 \times 10^{18} \text{ m}^{-3}$$

### ★ Dislocations—

$$1) \quad |\vec{b}_{Fe}| = 2 \times 0.124 \text{ nm} = 0.248 \text{ nm} \\ |\vec{b}_V| = 2 \times 0.205 \text{ nm} = 0.41 \text{ nm}$$

2) Clearly, the burgers' vectors will be

$$\vec{b}_1 = \frac{1}{4} [112] \quad \text{and} \quad \vec{b}_2 = \frac{1}{4} [11\bar{2}]$$

$$\text{Now, } \frac{\mu}{2} \left[ 2 \times \frac{1}{16} (1^2 + 1^2 + 2^2) - \frac{1}{4} (1^2 + 1^2 + 0^2) \right]$$

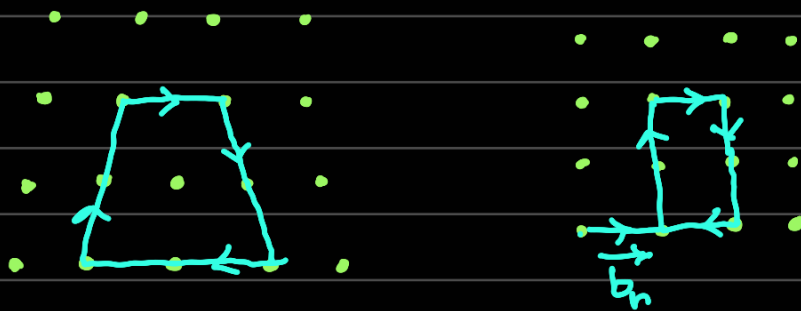
$$= \frac{\mu}{16} (6 - 4) = \frac{\mu}{8} > 0$$

$\therefore$  **non-spontaneous**

3.) Positive edge dislocation:



Negative edge dislocation:



Burgers' vectors are shown in the figures.  
we find  $\vec{b}_p + \vec{b}_n = 0$

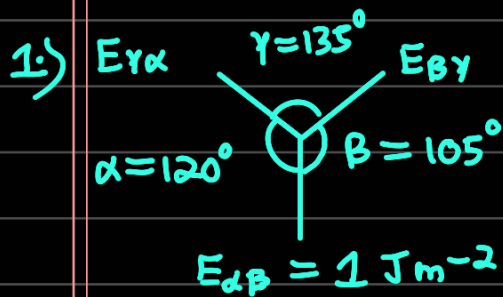
4.) Dislocation energy density  $= \frac{1}{2} G b^2 \rho$

$$= \frac{1}{2} \times 45 \times 10^9 \times \left( \frac{3.61}{\sqrt{2}} \times 10^{-10} \right)^2 \times 10^{10}$$

$\text{J m}^{-3}$

$$\approx 14.66 \text{ J m}^{-3}$$

# ☆ Surfaces and Grain Boundaries -



From Lamé's Theorem,

$$\frac{E_{\alpha\beta}}{\sin \gamma} = \frac{E_{\beta\gamma}}{\sin \alpha} = \frac{E_{\gamma\alpha}}{\sin \beta}$$

$$\text{So } E_{\beta\gamma} = \frac{\sin 120^\circ}{\sin 135^\circ} = \frac{\sqrt{3}/2}{1/\sqrt{2}} \approx \underline{1.22 \text{ J m}^{-2}}$$

$$E_{\gamma\alpha} = \frac{\sin 105^\circ}{\sin 135^\circ} = \frac{(\sqrt{3}+1)/2\sqrt{2}}{1/\sqrt{2}} \approx \underline{1.366 \text{ J m}^{-2}}$$

$$\begin{aligned} 2.) \text{ No. of grains per unit volume} &= \frac{1}{\frac{4}{3}\pi\left(\frac{d}{2}\right)^3} \\ &= \frac{6}{\pi d^3} \end{aligned}$$

$$\begin{aligned} \text{Grain boundary area per unit volume} \\ &= 4\pi\left(\frac{d}{2}\right)^2 \times \frac{6}{\pi d^3} = \frac{6}{d} \end{aligned}$$

If  $\gamma \rightarrow$  Grain boundary energy per unit area ( $\text{J m}^{-2}$ )

$$\text{Energy per unit volume, } E = \frac{6\gamma}{d}$$

If  $d$  increases,  $E$  decreases  $\Rightarrow \Delta E < 0$

$\Rightarrow$  Spontaneous process.

$$\Delta E = 6\gamma \left( \frac{1}{0.1 \times 10^{-3}} - \frac{1}{0.01 \times 10^{-3}} \right) \text{ J m}^{-3}$$

$$= -5.47 \times 10^5 \text{ J m}^{-3}$$

$$= -0.547 \text{ MJ m}^{-3}$$

3) wrong formula in question. It is actually

$$N = 2^{n-1} \Rightarrow n = 1 + \log_2 N$$

$$\text{Put } N = 45$$

$$\text{so } n = 1 + \log_2 45$$

$$= 1 + 5.492$$

$$= 6.492$$

—————x—————