3.091 Fall Term 2004

Homework #8

Solutions

1. $n_v/N = 3.091 \times 10^{-5}$ at 1234°C = 1507 K

$= 5.26 \times 10^{-3}$ at mp = 2716 K

$$\frac{n_v}{N} = A\ \exp\left(-\frac{\Delta H_v}{RT}\right)$$

$$3.091 \times 10^{-5} = A\ \exp - \frac{\Delta H_v}{1507\ R} \qquad (1)$$

$$5.26 \times 10^{-3} = A\ \exp - \frac{\Delta H_v}{2716\ R} \qquad (2)$$

$$(1)/(2) = 5.876 \times 10^{-3} = \exp\left(-\frac{\Delta H_v}{1507\ \ R} + \frac{\Delta H_v}{2716\ \ R}\right)$$

Taking the logarithm of both sides gives

$$-5.137 = \frac{\Delta H_v}{R}\left(-\frac{1}{1507} + \frac{1}{2716}\right) = -2.954 \times 10^{-4}\ \frac{\Delta H_v}{R} \Rightarrow \Delta H_v = 1.497 \times 10^5\ \text{J/mol}$$

2θ	**$\sin^2\theta$**	**normalized**	**clear fractions**	**(hkl)?**	$\frac{\sin^2\theta}{h^2+k^2+l^2}$
38.40	0.108	1.00	3	111	0.0360
44.50	0.143	1.32	4	200	0.0358
64.85	0.288	2.67	8	220	0.0359
77.90	0.395	3.66	11	311	0.0358
81.85	0.429	3.97	12	222	0.0358
98.40	0.573	5.31	16	400	0.0358
111.20	0.681	6.31	19	331	0.0358

2. All we need to know is the temperature dependence of the vacancy density:

$$\frac{n_v}{N} = Ae^{-\frac{\Delta H_v}{RT}}$$ where T is in Kelvins and the m.p. of Al is 660ºC

$$\frac{0.08}{100} = Ae^{-\Delta H_v/RT_1}$$, where T_1 = 923K; $$\frac{0.01}{100} = Ae^{-\Delta H_v/RT_2}$$, where T_2 = 757K

Taking the ratio:

$$\frac{8\times10^{-4}}{1\times10^{-4}} = \frac{Ae^{-\Delta H_v/RT_1}}{Ae^{-\Delta H_v/RT_2}} = e^{-\frac{\Delta H_v}{R}\left(\frac{1}{T_1}-\frac{1}{T_2}\right)} \qquad \therefore \ln 8 = -\frac{\Delta H_v}{R}\left(\frac{1}{T_1}-\frac{1}{T_2}\right)$$

$$\therefore \Delta H_v = -\frac{R\times\ln 8}{\frac{1}{923}-\frac{1}{757}} = -\frac{8.314\times\ln 8}{\frac{1}{923}+\frac{1}{757}} = 7.28\times10^4 \text{ J/mole vac}$$

$$\therefore \Delta H_v = \frac{7.28\times10^4}{6.02\times10^{23}} = 1.21\times10^{-19} \text{ J/vac} = 0.755 \text{ eV/vac}$$

3.(a) We need to know the temperature dependence of the vacancy density:

$$\frac{1}{10^4} = Ae^{-\frac{\Delta H_v}{kT_1}} \quad \text{and} \quad \frac{1}{10^3} = Ae^{-\frac{\Delta H_v}{kT_x}}$$

From the ratio: $$\frac{\frac{1}{10^4}}{\frac{1}{10^3}} = \frac{10^3}{10^4} = \frac{Ae^{-\Delta H_v/kT_1}}{Ae^{-\Delta H_v/kT_x}}$$ we get $$-\ln 10 = -\frac{\Delta H_v}{k}\left(\frac{1}{T_1}-\frac{1}{T_x}\right)$$

$$\therefore \left(\frac{1}{T_1}-\frac{1}{T_x}\right) = \frac{k\ln 10}{\Delta H_v}$$

$$\frac{1}{T_x} = \frac{1}{T_1} - \frac{k\ln 10}{\Delta H_v} = \frac{1}{1073} - \frac{1.38\times10^{-23}\times\ln 10}{2\times1.6\times10^{-19}} = 8.33\times10^{-4}$$

T_x = 1200 K = 928°C

(b) repeat the calculation following the method given above but with ΔH_v = 1.0 eV to find that T_x = 1364 K = 1091ºC

NOTE: the change in ΔH_v from 2.0 eV to 1.0 eV resulted in a change from 128 K to 291 K in ΔT.

4. Cu is FCC; example: (111) $[10\bar{1}]$; (111) $[\bar{1}01]$; $(\overline{111})$ $[0\bar{1}1]$; $(11\bar{1})$ $[\bar{1}01]$

5.

Defect	Type	Improved Materials Properties	Adversely Affected Materials Properties
	Vacancy f(T)	– diffusivity	– electron mobility

		– color centers – ionic conductivity	– carrier lifetime
Point Defect	Substitutional	– conductivity (dopant) – strength (hardness) – characteristic T (like T_M)	– conductivity (impurities) – ductility – characteristic T
	Interstitial	– strength – characteristic T – electrical properties	– ductility – characteristic T – electrical properties
Line Defect	Dislocation	– ductility (malleability) – strength (at high dislocation density)	– strength – yield stress – optical properties – lasing action
Planar Defect	Grain Boundaries	– strength	– creep resistance – electrical properties – magnetic properties

6. $\frac{n_v}{N} = A\exp -\frac{\Delta H_v}{k_B T}$, $\quad \Delta H_v = 1.5\,eV \quad \frac{n_v}{N} = \frac{1}{10^6}$ at 888°C

need first to solve for value of A -- use data at 888°C

$$A = \frac{\frac{n_v}{N}}{\exp -\frac{\Delta H_v}{k_B T}} = \frac{10^{-6}}{\exp -\frac{1.5\times 1.6\times 10^{-19}}{1.38\times 10^{-23}\times(888+273)}} = 3.203$$

calculate $\frac{n_v}{N}$ at m.p. of Pd, 1825 K

$$\therefore \frac{n_v}{N} = 3.203\times\exp\left(-\frac{1.5\times 1.6\times 10^{-19}}{1.38\times 10^{-23}\times 1825}\right) = 2.328\times 10^{-4} < 10^{-3}$$

$\therefore$ it is **not** possible to achieve a vacancy fraction of 10^{-3} by simply raising temperature.