Birla Institute of Technology and Science, Pilani
CHE F243 Materials Science and Engineering

II Semester 2014-15 | Mid Sem (Open Book)
Max Time: 90 min | Total Max Marks:105 | Date 13th March, 2015

SECTION B (65 marks)

Marks will be awarded only based on the concept

Q1: The planar density of the (112) plane in BCC iron is 9.94×10^{14} atoms/cm^2. Calculate the planar density and interplanar distance of the (110) and (100) planes. From your calculation, order these three from most to least preferred slip planes. **[10]**

Sol^n The lattice parameter of BCC iron is 0.2866 nm.

Planar density (110) = $\frac{\text{atoms}}{\text{area}} = \frac{2}{(\sqrt{2})(2.866\times10^{-8}\text{cm})^2} = 1.72\times10^{15}$ atom/cm^2 → 1.5

Planar density (112) = 9.94×10^{14} atoms/cm^2 (given)

Planar density (100) = 1.217×10^{15} atoms/cm^2. → 1.5

In terms of PD
110 > 100 > 112

Interplanar spacings are: $d_{110} = \frac{2.866\times10^{-8}}{\sqrt{1^2+1^2+0^2}} = 2.0266\times10^{-8}$ cm → 1.5

$d_{112} = \frac{2.866\times10^{-8}}{\sqrt{1^2+1^2+2^2}} = 1.17\times10^{-8}$ cm → 1.5

In terms of I/P
100 > 110 > 112 ← 0.5

$d_{100} = \frac{2.866\times10^{-8}}{\sqrt{1^2+0^2+0^2}} = 2.866\times10^{-8}$ cm → 1.5

Least preferred (112) and the other two planes, we cannot predict from this available data → 2

$\sqrt{3}a = 4R$

Q2: Determine the density of vacancies per cm^3 needed for a BCC iron crystal to have a theoretical density of 7.87 gm/cc. At room temperature iron lattice parameter is 2.866×10^{-8} cm. **[12]**

Sol^n Since the iron is BCC, 2 iron atoms are present in each unit cell.

$\rho = \frac{(2\text{ atoms/cell})(55.847\text{ g/mol})}{(2.866\times10^{-8}\text{cm})^3(6.02\times10^{23}\text{ atoms/mol})} = 7.8814$ g/cm^3 → 2

Calculating no. of iron atoms & vacancies that would be present in each unit cell for the required density of 7.87 g/cm^3.

$\rho = \frac{(x\text{ atoms/cell})(55.847\text{ g/mol})}{(2.866\times10^{-8}\text{cm})^3(6.02\times10^{23}\text{ atoms/mol})} = 7.87$ g/cm^3 → 2

$x\ \frac{\text{atoms}}{\text{cell}} = \frac{7.87(2.866\times10^{-8})^3(6.02\times10^{23})}{55.847} = 1.9971$ → 2

So, $2 - 1.9971 = 0.0029$ vacancies per unit cell. → 3

The number of vacancies per cm^3 is:

vacancies/cm^3 = $\frac{0.0029\text{ vacancies/cell}}{(2.866\times10^{-8}\text{cm})^3} = 1.23\times10^{20}$ → 3

Q3: Above 882 °C, Titanium has a BCC crystal structure, with a= 0.332 nm. Below 882 °C, it has an HCP crystal structure with a = 0.2978 nm and c = 0.4735 nm. Determine the % volume change when Titanium cool down from 883 °C to 881 °C. **[10]**

Initial (883°C) State $\xrightarrow[\text{BCC} \mid \text{HCP}]{882°C}$ Final (881°C) State

volume for BCC = a^3 = 0.036594 nm^3 → 2

volume for HCP = $1.5a^2c\sqrt{3}$ = 2.598 × 0.2978^2 × 0.4735 = 0.10909 nm^3

2

% change in volume = $\frac{\text{final vol} - (\text{Initial vol} \times 3)}{(3 \times \text{Initial vol})} \times 100$

BCC cell has 2 atoms/cell

= $\frac{0.10909 - 0.036594 \times 3}{0.036594 \times 3} \times 100$ → 2

HCP has 6 atoms/cell 2

= −0.63 (contraction) → 2

Q4: We have a LDPE sample containing 4000 chains with molecular weights between 0 and 5000 gm/mol, 8000 chains with molecular weights between 5000 and 10000 gm/mol, 7000 chains with molecular weights between 10000 and 15000 gm/mol, and 2000 chains with molecular weight between 15000 and 20000 gm/mol. Determine number and weight average molecular weight, PDI, and corresponding degree of polymerizations. **[12]**

Sol^n

Number of Chains (N_i)	Mean per chain ($\bar{M}_i$)	$x_i = \frac{N_i}{\Sigma N_i}$ (2)	$x_i\bar{M}_i$ (1.5)	Weight (W_i) $W_i = N_i \times \bar{M}_i$ (2)	$f_i = \frac{W_i}{\Sigma W_i}$ (1.5)	$f_i\bar{M}_i$ (2)
4000	2500	0.191	477.5	10×10^6	0.0519	129.75
8000	7500	0.381	2857.5	60×10^6	0.3118	2338.50
7000	12,500	0.333	4162.5	87.5×10^6	0.4545	5681.25
2000	17,500	0.095	1662.5	35×10^6	0.1818	3181.50
$\Sigma N_i = 21{,}000$		$\Sigma x_i = 1.00$	$\Sigma x_i\bar{M}_i = 9160$	$\Sigma W_i = 192.5 \times 10^6$	$\Sigma f_i = 1$	$\Sigma f_i\bar{M}_i = 11.331$

$\bar{M}_n = \Sigma x_i\bar{M}_i = 9160$ g/mol → 1

$\bar{M}_w = \Sigma f_i\bar{M}_i = 11331$ g/mol → 1

PDI = $\frac{11331}{9160}$ = 1.237

Degree of Polymerization = $\frac{9160}{28}$ = 327.142 → 1

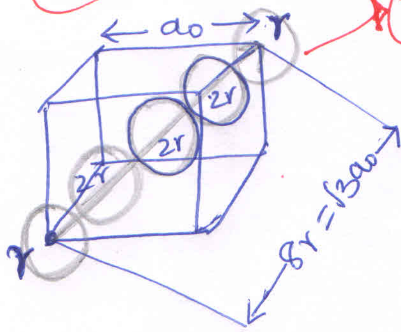
Q5: Derive the packing factor of silicon at room temperature with proper schematic. **[10]**

As in the figure we can find that atoms touch along the body diagonal of the cell. There are voids that have same diameter as atoms.

$$\sqrt{3}a_0 = 8r \quad 3$$

$$\text{Packing factor} = \frac{(8\ \text{atoms/cell})(\tfrac{4}{3}\pi r^3)}{(a_0)^3} \quad 3$$

$$= \frac{8 \times \frac{4}{3}\pi r^3}{(8r/\sqrt{3})^3}$$



2

So, Packing factor = 0.34 → 2

○ – Atoms

○ – voids

Q6: Consider the gas carburizing of a gear of 1020 steel at 927 °C. Calculate the time in minutes necessary to increase C content to 0.4 % at 0.5 mm below the surface. Assume that the C content at the surface is 0.9% . The normal C content of the steel is 0.2%. What will be the C content of the same place after 5 h of carburizing time? **[11]**

Sol^n Using Table 6.2 and interpolating: $D_{927°C} = 1.44 \times 10^{-11}\ m^2/s$ → 2

$$\frac{C_s - C_x}{C_s - C_0} = \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \; ; \quad C_s = 0.90\%,\ C_0 = 0.20\%,\ C_x = 0.40\% \; ; \quad x = 0.5\,mm = 5 \times 10^{-4}\,m$$

Substituting values:

$$\frac{0.9 - 0.4}{0.9 - 0.2} = \text{erf}\left[\frac{5.0 \times 10^{-4}\,m}{2\sqrt{(1.44 \times 10^{-11}\,m^2/s)(t)}}\right]$$

$$\text{erf}\left(\frac{65.88}{\sqrt{t}}\right) = 0.7143$$

$$Z = \frac{65.88}{\sqrt{t}} \quad \text{then erf } Z = 0.7143 \to 1$$

From table 6.1 and interpolating (to find a number for Z whose ~~number~~ error function (erf) is 0.7143)

$$\frac{0.7143 - 0.7112}{0.7421 - 0.7112} = \frac{y - 0.75}{0.80 - 0.75} \to 2$$

erf Z	Z
0.7112	0.75
0.7143	y
0.7421	0.80

$$\Rightarrow y = 0.755 \to 1$$

then $Z = \frac{65.88}{\sqrt{t}} = 0.755$

$t = 7614\,s \simeq 127$ min

Same for 2nd Part

$$\frac{0.9 - C}{0.7} = \text{erf } 0.49 \simeq 0.5$$

$C \simeq 0.55\%$ → 3H