

# Exam I

Wednesday, 21 March, 2007

Duration: 50 minutes

Closed Book Exam

Write clearly your derivations and answers on the question sheet

Name:

ID#:

## I Diffusion [30 points]

- Calculate the diffusion coefficient of carbon in (i) Austenite and (ii) Ferrite (of steel) at 920°C. Use your knowledge to explain the difference between the two values.
- A mild steel component (carbon content 0.2%) is to be case-hardened by placing it in a furnace in an atmosphere rich in hydrocarbon gas so that the surface concentration is 0.8% carbon. The design of the component requires that at the completion of this process, the carbon concentration at 1 mm below the surface will be 0.55%. The furnace is set at 1050°C. Determine the time required for the heat treatment.

EXAM I SOLUTION:

I] a)  $D = D_0 e^{-\frac{Q_d}{RT}}$

i)  $\gamma$  (Fe)  $T = 900^\circ\text{C}$   $Q_d = 148 \text{ kJ/mol}$   
 $D_0 = 2.3 \times 10^{-5} \text{ m}^2/\text{s}$   
 $T = 1173 \text{ K}$

$$D_1 = 2.3 \times 10^{-5} e^{-\left(\frac{148 \times 10^3}{8.31 \times 1173}\right)} = 5.858 \times 10^{-12} \text{ m}^2/\text{s}$$

ii)  $\alpha$  (Fe)  $T = 900^\circ\text{C}$   $Q_d = 80 \times 10^3$   
 $D_0 = 6.2 \times 10^{-7} \text{ m}^2/\text{s}$   
 $T = 1173$

$$\Rightarrow D_2 = 6.2 \times 10^{-7} e^{-\left(\frac{80 \times 10^3}{8.31 \times 1173}\right)} = 1.65 \times 10^{-10} \text{ m}^2/\text{s}$$

$D_1 < D_2 \Rightarrow$  diffusion occurs at a lower rate in  $\gamma$  Fe because it has FCC that is more packed than BCC.

b)  $C_0 = 0.2 \text{ wt}\%$   
 $C_s = 0.8 \text{ wt}\%$  ( $x = 0.55 \text{ wt}\%$ )  
 $x = 1.0 \times 10^{-3} \text{ m}$   
 $T = 1323 \text{ K}$

$$\frac{C_x - C_0}{C_s - C_0} = 1 - \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \Rightarrow 1 - \left(\frac{0.55 - 0.2}{0.8 - 0.2}\right) = \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

$$\Rightarrow 0.4167 = \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

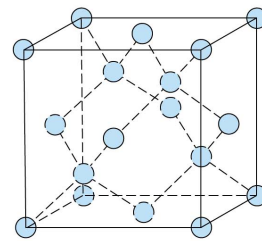
Using table  $\Rightarrow Dxt = 1.111 \times 10^6$

At  $T = 1323 \text{ K}$   $D = 2.3 \times 10^{-5} e^{-\left(\frac{148 \times 10^3}{1323 \times 8.31}\right)}$   
 $\Rightarrow \alpha$  Fe  $= 3.276 \times 10^{-11}$

$$\Rightarrow t = \underline{\underline{14.08 \text{ h}}}$$

## II Microstructures [40 points]

- Draw the following directions and planes in a FCC unit cell  
(110) (112) [121] [-121]  
List all the members in the  $\langle 122 \rangle$  family
- Calculate the planar packing density of the (110) plane in FCC structure
- Pure iron undergoes an allotropic phase transformation from FCC (austenite) to BCC (ferrite) on cooling at  $910^{\circ}\text{C}$ . Calculate the percent change in volume accompanying this transformation assuming that the atom diameter is the same in both structures
- Calculate the density of silicon given that its atomic mass is 28.086 amu, its lattice parameter,  $a$ , is 0.543 nm, its crystal structure is diamond cubic.



diamond cubic crystal structure

### **III Microstructures [30 points]**

- a. One of the tetrahedral interstitial sites in the BCC structure locates at position  $(1/2, 1/4, 0)$ .  
Using a sketch to identify all the tetrahedral interstitial sites in a BCC unit cell. How many (whole) tetrahedral sites are in this unit cell?
- b. What is the atom-to-interstitial site ratio for the tetrahedral interstitial sites in the BCC structure?
- c. What is the size, relative to that of the atoms, of the tetrahedral interstitial sites in BCC?

# Data and Formula

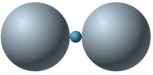
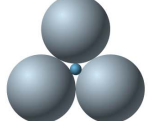
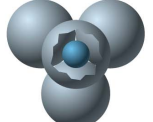
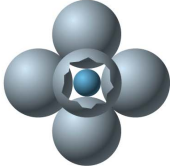
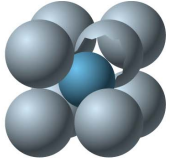
Avogadro's number:  $6.023 \times 10^{23}$  /mol

Gas Constant:  $8.31 \text{ J/mol} \cdot \text{K}$ ,  $1.987 \text{ cal/mol} \cdot \text{K}$

Boltzmann's constant:  $1.38 \times 10^{-23} \text{ J/atom} \cdot \text{K}$ ,  $8.62 \times 10^{-5} \text{ eV/atom} \cdot \text{K}$

**Table 5.1** Tabulation of Error Function Values

$z$	$\text{erf}(z)$	$z$	$\text{erf}(z)$	$z$	$\text{erf}(z)$
0	0	0.55	0.5633	1.3	0.9340
0.025	0.0282	0.60	0.6039	1.4	0.9523
0.05	0.0564	0.65	0.6420	1.5	0.9661
0.10	0.1125	0.70	0.6778	1.6	0.9763
0.15	0.1680	0.75	0.7112	1.7	0.9838
0.20	0.2227	0.80	0.7421	1.8	0.9891
0.25	0.2763	0.85	0.7707	1.9	0.9928
0.30	0.3286	0.90	0.7970	2.0	0.9953
0.35	0.3794	0.95	0.8209	2.2	0.9981
0.40	0.4284	1.0	0.8427	2.4	0.9993
0.45	0.4755	1.1	0.8802	2.6	0.9998
0.50	0.5205	1.2	0.9103	2.8	0.9999

Coordination Number	Cation-Anion Radius Ratio	Coordination Geometry
2	< 0.155	
3	0.155-0.225	
4	0.225-0.414	
6	0.414-0.732	
8	0.732-1.0	

**Table 5.2** A Tabulation of Diffusion Data

Diffusing Species	Host Metal	$D_0(\text{m}^2/\text{s})$	Activation Energy $Q_d$		Calculated Values	
			$\text{kJ/mol}$	$\text{eV/atom}$	$T(^{\circ}\text{C})$	$D(\text{m}^2/\text{s})$
Fe	$\alpha$ -Fe (BCC)	$2.8 \times 10^{-4}$	251	2.60	500	$3.0 \times 10^{-21}$
					900	$1.8 \times 10^{-15}$
Fe	$\gamma$ -Fe (FCC)	$5.0 \times 10^{-5}$	284	2.94	900	$1.1 \times 10^{-17}$
					1100	$7.8 \times 10^{-16}$
C	$\alpha$ -Fe	$6.2 \times 10^{-7}$	80	0.83	500	$2.4 \times 10^{-12}$
					900	$1.7 \times 10^{-10}$
C	$\gamma$ -Fe	$2.3 \times 10^{-5}$	148	1.53	900	$5.9 \times 10^{-12}$
					1100	$5.3 \times 10^{-11}$
Cu	Cu	$7.8 \times 10^{-5}$	211	2.19	500	$4.2 \times 10^{-19}$
Zn	Cu	$2.4 \times 10^{-5}$	189	1.96	500	$4.0 \times 10^{-18}$
Al	Al	$2.3 \times 10^{-4}$	144	1.49	500	$4.2 \times 10^{-14}$
Cu	Al	$6.5 \times 10^{-5}$	136	1.41	500	$4.1 \times 10^{-14}$
Mg	Al	$1.2 \times 10^{-4}$	131	1.35	500	$1.9 \times 10^{-13}$
Cu	Ni	$2.7 \times 10^{-5}$	256	2.65	500	$1.3 \times 10^{-22}$

**Source:** E. A. Brandes and G. B. Brook (Editors), *Smithells Metals Reference Book*, 7th edition, Butterworth-Heinemann, Oxford, 1992.