

# Exam I

Wednesday, 30 March, 2005

Duration: 60 minutes

Closed Book Exam

Write clearly your derivations and answers on the question sheet

Name:

ID#:

## **I Diffusion [25 points]**

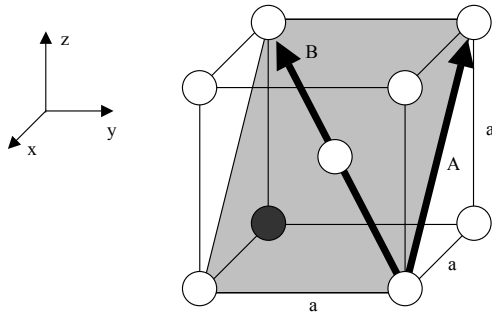
- a. Calculate the diffusion coefficient of carbon in (i) Austenite ( $\gamma$ -Fe) and (ii) Ferrite ( $\alpha$ -Fe) at 900°C. Use your knowledge to explain the difference between the two values.
- b. A mild steel component (carbon content 0.2%) is to be case hardened by placing it in a furnace in an 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.

## **II Microstructures [25 points]**

Given the fact that platinum (Pt) is FCC with atomic weight 195, calculate the mass of one unit cell. Then, given the density =  $21.5 \text{ g/cm}^3$ , calculate the size of the unit cell and the diameter of a Pt atom. Finally, calculate the planar density of packing of Pt atoms on a close-packed (111) plane. (Consider the plane to pass through the centers of the atoms.)

### III Crystal Structure [30 points]

Shown below is a body centered cubic unit cell



- Write down the miller indices of the shaded plane according to the atomic coordinate system given (pay attention to the style of notation of indices for planes)
- Write down the indices of ALL other planes belonging to the same plane family with this plane
- Calculate the planar packing density of this plane (show your calculation procedure)
- Write down the indices of direction A and direction B (pay attention to the style of notation of indices for directions)
- Is this plane a slip plane? if not identify a slip plane. Are directions A and B, or either of them slip directions? if not identify a slip direction. How many slip directions are there on this plane (you do not need to mark them out)? How many slip systems in total in this structure (you do not need to mark them out)?
- Determine the magnitude of Burgers vector in this structure (show your calculations if any)



## **IV Ceramics [20 points]**

Some hypothetical ceramic compound has the chemical formula  $A_2BO_4$  in which both A and B are cations. The  $O^{2-}$  ions form a hexagonal close-packed structure and the  $A^{3+}$  and  $B^{2+}$  ions occupy tetrahedral and/or octahedral positions (to be determined). The atomic radii of the  $A^{3+}$ ,  $B^{2+}$  and  $O^{2-}$  ions are 0.041, 0.052 and 0.140 nm, respectively.

- a. Determine the site type(s) (i.e. tetrahedral, octahedral) that the  $A^{3+}$  and  $B^{2+}$  ions occupy.
- b. What fractions of the site types is occupied with the  $A^{3+}$  and with the  $B^{2+}$  ions (for number of tetrahedral and octahedral sites in HCP structure see provided table)

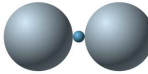
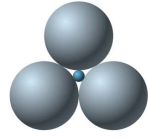
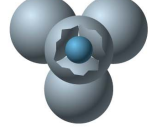
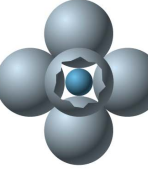
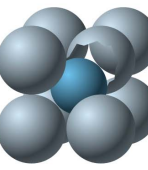
# Data and Formula

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

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

**Table 5.1** Tabulation of Error Function Values

$z$	$erf(z)$	$z$	$erf(z)$	$z$	$erf(z)$
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	$D_0(m^2/s)$	Activation Energy $Q_d$		Calculated Values	
			$kJ/mol$	$eV/atom$	$T(^{\circ}C)$	$D(m^2/s)$
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.

Crystal Structure	Size of Tetrahedral Sites	Size of Octahedral Sites	Number of Tetrahedral Sites per Unit Cell (per Host Atom)	Number of Octahedral Sites per Unit Cell (per Host Atom)
BCC	$r/R=0.291$	$r/R=0.155$	12 (6)	6 (3)
FCC	$r/R=0.225$	$r/R=0.414$	8 (2)	4 (1)
HCP	$r/R=0.225$	$r/R=0.414$	12 (2)	6 (1)