National Exams May 2003

98 – Met - A4, Structure of Materials

3 Hours duration

NOTES:

1. If doubt exists as to the interpretation of any question, the candidate is urged to submit with the answer paper, a clear statement of any assumptions made;

2. Candidates may use one of two calculators, the Casio or Sharp approved models. This is a Closed Book exam. All equations, constants and diagrams are given in the appendix.

3. **Any five** questions constitute a complete paper. **Only the first five questions** as they appear in your answer book will be marked.

4. All questions are of equal value.

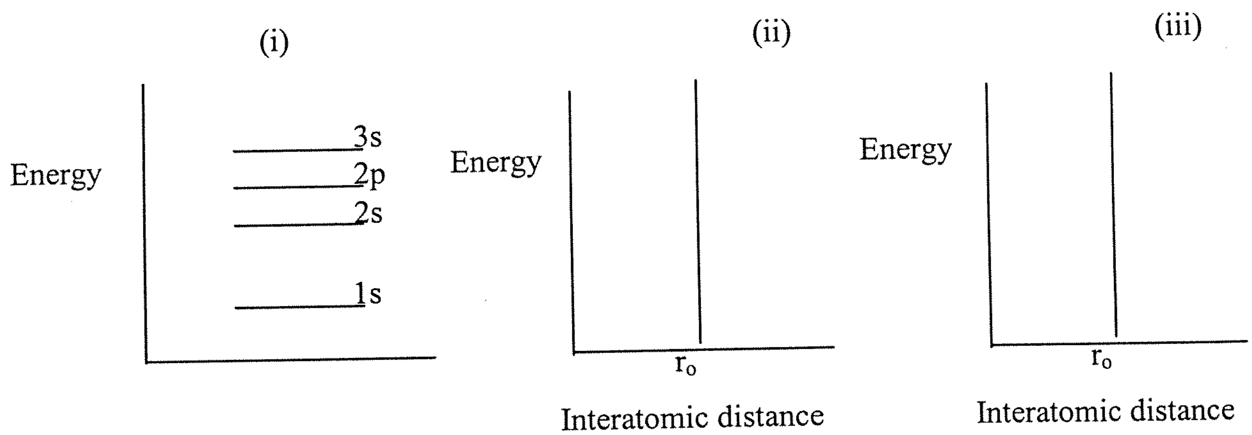
QUESTION I. ELECTRON STRUCTURE, BAND STRUCTURE, INTERATOMIC BONDING

4 marks 1) Magnesium has an atomic number of 12. Write down the electron configuration of Mg.

5 marks 2) Write down the quantum numbers for all electrons in a Mg atom in a table as shown below.

n	**l**	m_l	m_S
1	0	0	± 1/2
2			
2			
2			
2			
3			

5 marks 3) The energy diagram for an **individual** atom of Mg is given in Fig. (i) below. When a solid cluster of 6 Mg atoms is formed, the interatomic distance becomes important. Prepare a figure as illustrated in Fig. (ii) below, indicating the change to the energy diagram necessary for 6 atoms. Finally, prepare another figure (such as Fig. iii below) showing the changes required when one has a system of N atoms (e.g. N= 1 mol).



6 marks 4) In the table below indicate what type of bonding occurs in each of the different materials.

Material	Type of Bonding
Al	
NaCl	
Si	
Al_2O_3	
Nylon	
Pb-Sn solder	

QUESTION II. CERAMIC STRUCTURE AND FLEXURAL STRENGTH

1) Barium titanate ($BaTiO_3$) is listed as a cubic ABX_3 perovskite structure with coordination numbers of 12 for Ba^{2+}, 6 for Ti^{4+} and 6 for O^{2-}, respectively. The anion packing forms an FCC arrangement (while the entire structure is simple cubic with one ($BaTiO_3$) formula unit per lattice point).

6 marks a) In a cubic unit cell draw the positions of all Ba^{2+}, Ti^{4+} and O^{2-} ions. Use different colors or symbols to clearly distinguish between the different species in the unit cell.

8 marks b) The atomic weights for the different species in $BaTiO_3$ are as follows: A_{Ba} = 137 amu, A_{Ti} = 48 amu and A_O = 16 amu. The density of $BaTiO_3$ is 6 g/cm^3. Calculate the lattice parameter for the unit cell shown above.

6 marks 2) In a three point bending test the force at fracture of a ceramic brick (L = 178 mm, b = 114 mm, d = 76 mm) was 7 x 10^4N. For another brick made of the same material with the same flexural strength (=modulus of rupture or fracture strength) and having the same length (**L**) and width (**b**), but a height (**d**) of only 64 mm, calculate the load necessary to break the thinner brick.

QUESTION III. X-RAY DIFFRACTION

Iron has a body centered cubic structure with a lattice parameter of $a = 2.86 \times 10^{-10}$ m.

16 marks 1) Calculate the 2θ values for the first four diffraction peaks that would be obtained in an X-ray diffraction run for an iron powder sample using Cu - K_α radiation ($\lambda = 1.542 \times 10^{-10}$ m). Consult the reflection rules in the appendix to determine the Miller indices for these planes.

4 marks 2) Using four different cubic unit cells draw all four planes determined in part 1).

QUESTION IV. EQUILIBRIUM PHASE DIAGRAMS

The binary Fe-C phase diagram is shown in the appendix.

6 marks 1) Determine the temperatures and compositions of all invariant reactions in this system. Write down the phase reaction associated with each of the invariant reactions.

4 marks 2) For liquid steel containing 2.5 wt% C determine the following:

a) When the steel is slowly cooled at what temperature would the first crystals form?

b) What is the composition of the first crystals to form?

c) At what temperature would the last liquid solidify?

d) What is the composition of the last liquid to solidify?

6 marks 3) For a steel containing 1 wt%C draw the equilibrium microstructures that would be observed at:

b. 1000^0C

c. 750^0C

d. 500^0C

Label all phases in your microstructures.

4 marks 4) Determine the quantities of the two phases for the structure at 500^0C for the same steel with 1 wt% C.

QUESTION V. CASE HARDENING

12 marks 1) A low carbon steel with 0.2%C is carburized in a hydrocarbon gas at 1000^0C. The surface of the steel reaches a value of 1%C very rapidly. Calculate the carbon content at a depth of 0.3 mm beneath the surface after 10 hrs at 1000^0C. The diffusion coefficient for C is Fe at 1000^0C is given as D=0.298 x 10^{-6} cm^2/sec.

8 marks 2) Calculate the time necessary to raise the carbon level at the same depth to 0.6%.

QUESTION VI. PLASTIC DEFORMATION AND SLIP IN BCC METALS

Plastic deformation in body centered cubic (bcc) crystals occurs by slip of dislocations along the {110} type planes in directions of closest packing on these planes. There are 6 non-parallel {110} type planes in the cube and 2 closed packed directions on each plane giving a total of 12 slip systems. (Remember that positive and negative slip directions are equivalent, they are only counted once).

16 marks 1) Prepare a table listing all (hkl) [uvw] pairs for the 12 possible slip systems.

4 marks 2) Draw a cubic unit cell showing the $(01\bar{1})$ slip plane. On this plane show the two possible slip directions and give their [uvw] values.

QUESTION VII. STRENGTHENING MECHANISMS IN METALS

14 marks 1) Reducing the grain size in a metal usually results in increasing hardness and yield strength. This is referred to as the Hall-Petch relationship.
For polycrystalline brass calculate the yield-strength that would be obtained at grain sizes of 1μm and 0.1μm, given the following information for brass samples with larger grain size:

Grain Size	Yield Strength
100 μm	60 MPa
10 μm	150 MPa

6 marks 2) List the other three technologically important strengthening mechanisms for metals and briefly describe how hardness/strength is increased in each of them.

QUESTION VIII. ELASTIC DEFORMATION

20 marks A cylindrical rod 120 mm long and having a diameter of 15.0 mm is to be deformed using a tensile lead of 35,000 N. It must not experience either plastic deformation or a diameter reduction of more than 1.2×10^{-2} mm. Of the materials listed below, which are possible candidates? Justify your choice(s).

Materials	Modulus of Elasticity (GPa)	Yield Strength (MPa)	Poisson's Ratio
Aluminum alloy	70	250	0.33
Titanium alloy	105	850	0.36
Steel alloy	205	550	0.27
Magnesium alloy	45	170	0.20

APPENDIX

TABLE OF THE ERROR FUNCTION

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

TABLE 3.7-1 Reflection Rules of X-Ray Diffraction for the Common Metal Structures

Crystal Structure	Diffraction Does Not Occur When:	Diffraction Occurs When:
Body-centered cubic (bcc)	$h + k + l$ = odd number	$h + k + l$ = even number
Face-centered cubic (fcc)	h, k, l mixed (i.e., both even and odd numbers)	h, k, l unmixed (i.e., are all even numbers or all odd numbers)
Hexagonal close packed (hcp)	$(h + 2k) = 3n$, l odd (n is an integer)	All other cases

APPENDIX

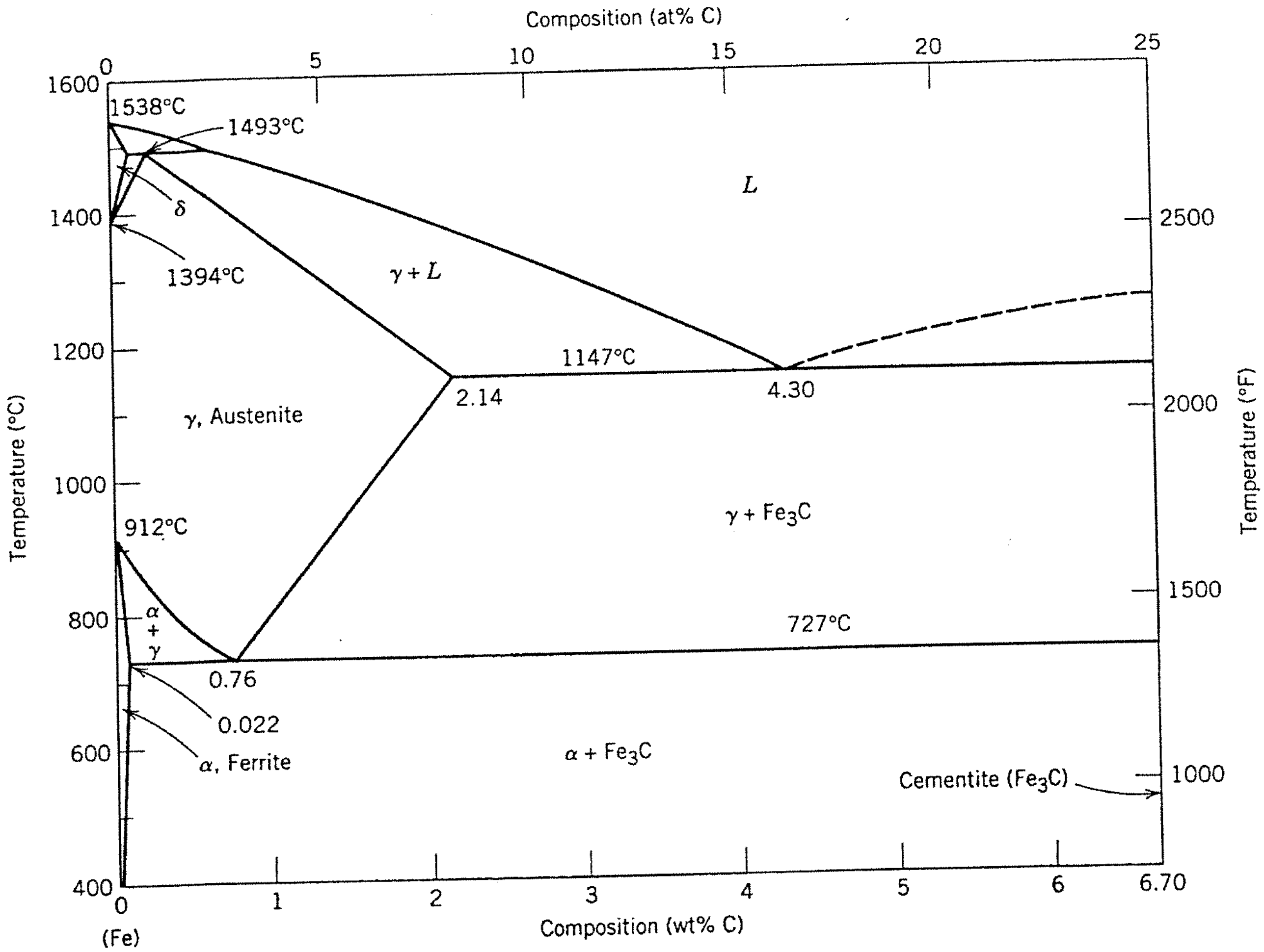


FIGURE 9.21 The iron–iron carbide phase diagram. [Adapted from *Binary Alloy Phase Diagrams,* 2nd edition, Vol. 1, T. B. Massalski (Editor-in-Chief), 1990. Reprinted by permission of ASM International, Materials Park, OH.]

Equations

Avogadro's number 6.023×10^{23} molecules / mol

Boltzmann's constant 1.38×10^{-23} J / atom-K

$n = 1, 2, 3, \ldots$

$l = 0, 1, 2, 3, \ldots n-1$

$m_l = 0, \pm 1, \pm 2, \pm 3, \ldots \pm l$

$m_s = \pm 1/2$

$$\rho = \frac{n' \left(\Sigma A_C + \Sigma A_A\right)}{V_C N_A}$$

$$\sigma = \varepsilon \cdot E$$

$$\sigma_{fs} = \frac{3F_f \cdot L}{2bd^2}$$

$$\sigma = F/A$$

$$\lambda = 2d \sin \theta$$

$$\nu = -\frac{\varepsilon_x}{\varepsilon_y}$$

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$1 MPa = 10^6 \ N/m^2$$

$$\frac{C_s - C_x}{C_s - C_o} = erf\left(\frac{x}{2\sqrt{Dt}}\right)$$

$$\sigma = \sigma_o + k \cdot d^{-1/2}$$