National Exams December 2012

98-Met-A4, Structure of Materials

3 Hours Duration

NOTES:

1. Attempt any **five** questions. **Only the first five** questions as they appear in your answer book will be marked.

2. All questions carry equal weightage (20 marks).

3. Candidates may use one of two calculators, the Casio or Sharp approved models. This is a CLOSED BOOK exam. All necessary equations, constants and diagrams are provided in the appendix.

4. If a 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.

Question I: Electron Structure and Bonding

1. Describe the set of quantum numbers that are needed to describe the electronic configuration of any element in the periodic table. What do each of the quantum numbers mean and what are their allowed values? State the electronic configuration of Titanium (Ti) with an atomic number of 22. **(5 marks)**

2. Differentiate between metallic and covalent bonding, while providing examples of each. Utilize diagrams to explain your answer. **(5 marks)**

3. Suppose the net potential energy between two atoms is given by: $E = \frac{A}{r^{12}} - \frac{B}{r^6}$, where r is the interatomic spacing and A , B are constants for a given material system. Derive an expression for the force between these two atoms, equilibrium interatomic spacing and the maximum binding energy. **(10 marks)**

Question II: Crystal Structure

1. Draw the following planes and directions (use separate drawings). **(8 marks)**
   a. Planes in cubic unit cells: $(1\bar{1}0)$, (221)
   b. Directions in hexagonal unit cells: $[1\bar{1}00]$, $[11\bar{2}0]$.

2. Copper has an FCC crystal structure and a unit cell with a lattice constant of 0.361 nm and an atomic weight of 63.5g/mol. **(3 parts of 4 marks each = Total 12 marks)**
   a. Compute its theoretical density, and compare with a measured value of 8.94 g/cm^3.
   b. What is its interplanar spacing d_{220}?
   c. Compute the planar density of a (110) plane.

Question III: Point Defects in Crystals

1. Point defects are present in every engineering material. Give one example where these defects are beneficial and one example where they are deleterious. Explain why? **(6 marks)**

2. Explain Schottky and Frenkel imperfections schematically. Give examples of material systems in which these defects may occur. **(6 marks)**

3. Calculate the equilibrium number of vacancies per m^3 for Copper at 1000°C. The energy for vacancy formation is 0.9 eV/atom; the atomic weight and density for copper are 63.5 g/mol and 8.4 g/cm^3 at this temperature. **(8 marks)**

Question IV: Diffusion

1. Differentiate between steady-state and nonsteady-state diffusion. Provide one example of each case. **(4 marks)**

2. How does the rate of diffusion change with operating temperature? Determine the ratio of diffusion rates of carbon in α-Fe (D_{T2}/D_{T1}) when T_1=500°C and T_2 = 900°C. The activation energy is 80 KJ/mol. **(8 marks)**

3. Consider the gas carburising of a steel alloy at 950°C with an initial carbon concentration of 0.25 wt%. If the carbon concentration at the surface is suddenly brought to and maintained at 1.20 wt%, how long will it take to achieve a carbon content of 0.80 wt% at a position 0.5 mm below the surface? The diffusion coefficient for carbon in iron at this temperature is 1.6×10^{-11} m^2/s; assume that the steel piece is semi-infinite. **(8 marks)**
   You might need the error function values provided in the following table:

Z	Erf(Z)
0.30	0.3286
0.35	0.3794
0.40	0.4284
0.45	0.4755
0.50	0.5205
0.55	0.5633
0.60	0.6039
0.65	0.6420
0.70	0.6778
0.75	0.7112
0.80	0.7421
0.85	0.7707
0.90	0.7969

Question V: Phase Diagram

For the binary eutectic phase diagram for iron-carbon (Fe-C) shown below, answer the following questions: **(5 parts of 4 marks each = Total 20 marks)**

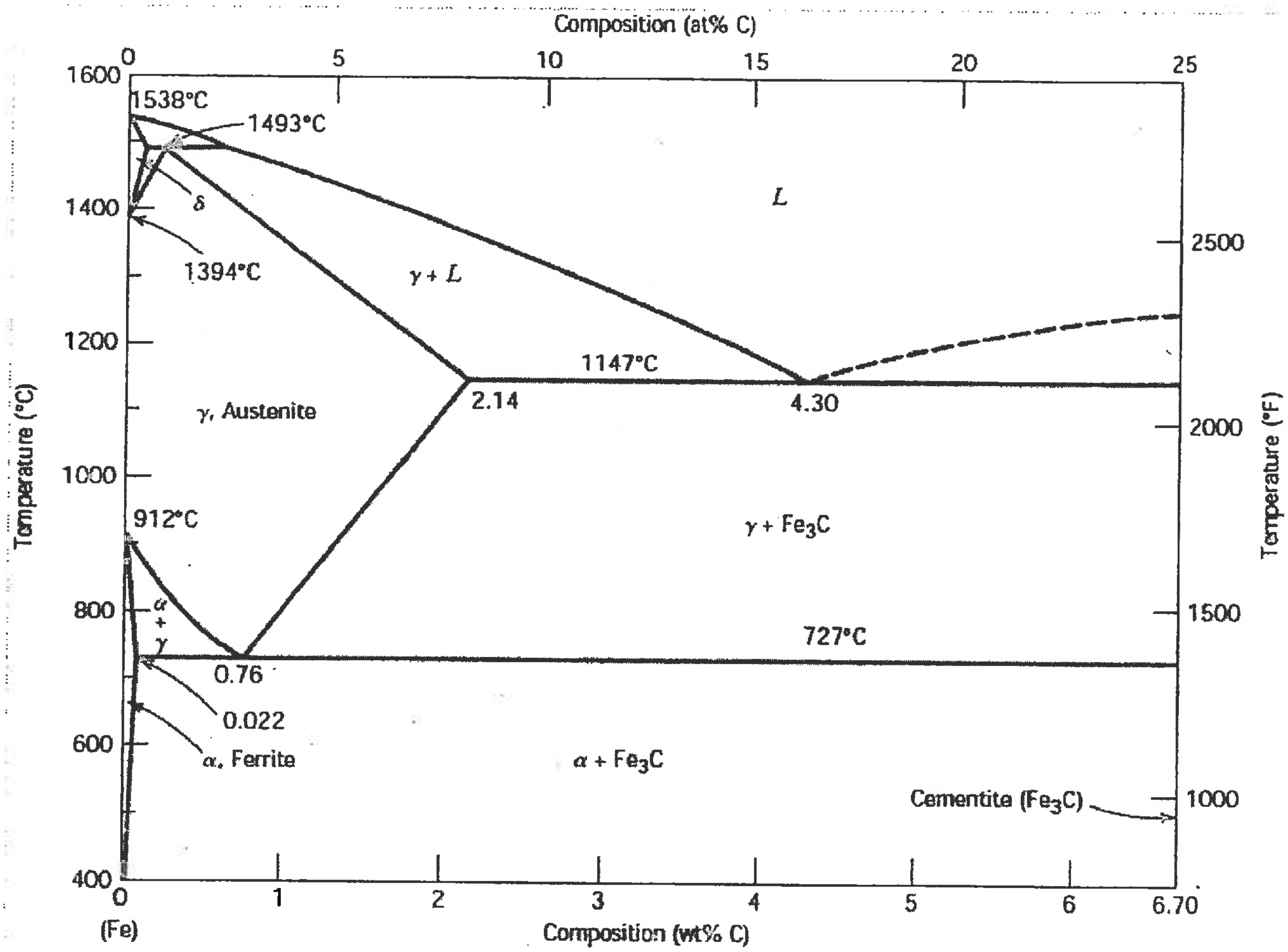

FIGURE 10.26 The iron–iron carbide phase diagram. (Adapted from *Binary Alloy Phase Diagrams*, 2nd edition, Vol. 1, T. B. Massalski, Editor-in-Chief, 1990. Reprinted by permission of ASM International, Materials Park, OH.)

1. What are the phases present at 2 wt% carbon content and a temperature of 1000°C?
2. Determine the maximum solubility of carbon in α-ferrite and austenite phases.
3. Explain the effect of increasing carbon content in iron on strength and ductility of the alloy system.
4. For a 99.65 wt% Fe-0.35 wt% C alloy at a temperature just below 727°C, determine the fractions of phases present.
5. Define eutectoid reaction. Write the eutectoid reaction for the Fe-C system.

Question VI: X-ray Diffraction and Microstructural Characterization

1. X-ray diffraction pattern of a sample of BCC iron occurred at $2\theta = 44.704°$ for $\{110\}$ planes. Calculate the lattice constant for the material if wavelength of the incoming ray was 0.1541 nm. At what angle of incidence will the diffraction peak for $\{211\}$ planes occur? **(10 marks)**

2. Give examples of two experimental techniques, other than the X-ray diffraction, that can be used to determine the microstructure of crystalline materials. Explain the underlying principles. **(10 marks)**

Question VII: Dislocations, Slip and Grain Boundaries

1. Does the metal strength decrease or increase when the average grain size is reduced. Why? **(4 marks)**

2. What is a slip system? What are the slip system for an FCC crystal? **(6 marks)**

3. Consider a zinc crystal being pulled in tension, with the normal to its basal plane (0001) at 60° to the tensile axis and with the slip direction $[11\bar{2}0]$ at 40° to the tensile axis.
   a. What is the resolved shear stress, τ, acting in the slip direction when a tensile stress of 0.69 MPa is applied? **(5 marks)**
   b. What tensile stress is necessary to reach the critical resolved shear stress, τc, of 0.94 MPa? **(5 marks)**

Question VIII: Mechanical Deformation

1. Consider a cylindrical brass rod with a diameter of 10 mm loaded in tension along its length. The Young's modulus and Poisson's ratio for brass are given as 97 GPa and 0.34, respectively. The yield strength and ultimate tensile strength of the material are 200 MPa and 550 MPa.
   a. Calculate the maximum load that the rod can sustain: (i) before yielding (P_{yield}), and (ii) before final failure (P_{max})? **(6 marks)**
   b. Determine the magnitude of the load required to produce a 2.5 μm reduction in diameter if the deformation is entirely elastic. **(8 marks)**
   c. If the material was loaded to a stress level of 300 MPa, and then unloaded fully, determine the amount of permanent residual strain in the material. **(6 marks)**

Appendix: Equations and constants

Avogadro's number	6.023×10^{23} molecules/mol
Boltzmann's constant (k)	1.38×10^{-23} J/atom-K = 8.62×10^{-5} eV/atom-K
Universal gas constant (R)	8.31 J/mol-K
1 MPa = 10^6 N/m^2	1 GPa = 10^9 N/m^2

$n = 1, 2, 3, \ldots$ $\quad l = 0, 1, 2, \ldots. n-1$ $\quad m_l = 0, \pm 1, \pm 2, \pm 3, \ldots.. \pm l$ $\quad m_s = \pm 1/2$

$$F = -\frac{\partial E}{\partial r}$$

$$E_n = -\frac{Z^2 R_E}{n^2} \qquad \Delta E = E_i - E_f = R_E\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) \qquad R_E = 13.61\,\text{eV}$$

$$N_D = N \exp\left(-\frac{Q_D}{kT}\right) \qquad N = \frac{\rho N_A}{A_{wt}};\ A_{wt} = \text{atomic weight}$$

$$a = 2R \qquad a = 2\sqrt{2}R \qquad a = \frac{4}{\sqrt{3}}R \qquad APF = \frac{V_s}{V_c} \qquad \rho = \frac{n.A_{wt}}{V_c.N_A}$$

$$T_K = T_C + 273 \qquad A = \pi r^2 \qquad V = \frac{4}{3}\pi R^3$$

$$n\lambda = 2d\sin\theta \qquad \frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}; \quad \text{if } a = b = c, \text{ then } d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$\frac{C_s - C_x}{C_s - C_0} = erf\left(\frac{x}{2\sqrt{Dt}}\right) \qquad D = D_0 \exp\left(-\frac{Q_d}{RT}\right)$$

$$\tau_R = \sigma.\cos\phi.\cos\lambda \qquad \sigma = \sigma_0 + k.d^{-1/2}$$

$$\varepsilon = \frac{\Delta l}{l_0} \qquad \sigma = \frac{F}{A_0} \qquad \sigma = E\varepsilon \qquad \tau = \frac{F}{A_0} \qquad \tau = G\gamma$$

$$E = 2G(1 + \upsilon) \qquad \nu = -\frac{\varepsilon_y}{\varepsilon_x} \qquad \%EL = 100\,\varepsilon_f$$