National Exams May 2013

98-Phys-B7, 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. Write down the electronic configurations of (a) Titanium, atomic number = 22, and (b) Iron, atomic number = 26. Explain why the 3d orbital gets filled earlier than the 4s orbital.
   (2 + 2 + 3 = 7 marks)

2. Diffentiate between the mechanical properties (such as hardness) of diamond and graphite. Based on their structure and chemical bonding, explain why is there a difference in the mechanical behavior of these two allotropes of Carbon. **(5 marks)**

3. (a) Compare the wavelength of an electron moving at 16.67 percent of the speed of light with that of a baseball with a mass of 0.142 kg traveling at 42.91 m/s. Assume wave-particle duality to hold for both particles. Electron mass is given as 9.11×10^{-31} kg. **(4 marks)**
   (b) In the above problem, if the uncertainty associated with the measurement of the speed of the baseball is 1 percent, then what is the corresponding uncertainty in knowing the position of the baseball? **(4 marks)**

Question II: Crystal Structure

1. Draw the following planes and directions (use separate drawings). **(8 marks)**
   (a) Planes in cubic unit cells: $(11\bar{1})$, (210)
   (b) Planes and directions in hexagonal unit cells: $(1\bar{1}00)$,$[11\bar{2}0]$

2. MgO has the NaCl type unit cell, in which alternate atomic positions in the FCC lattice are occupied by Mg^{2+} and O^{2-}. Draw this structure. If the ionic packing factor (IPF) is defined as the fraction of the unit-cell volume occupied by various cations and anions, calculate IPF for MgO. Also calculate its mass density in g/cm^3. **(6 + 6 = 12 marks)** The following data is provided:

   $r_{Mg^{2+}} = 0.078$ nm, $r_{O^{2-}} = 0.132$ nm, Molar masses: for Mg = 24.31 g, for O = 16 g.

Question III: Point Defects in Crystals

1. Differentiate between interstitial and substitutional solid solutions. What are the parameters that tend to enhance formation of substitutional solid solutions? **(6 marks)**

2. Calculate the radius of the largest interstitial void in the FCC γ-iron lattice. The atomic radius of the iron atom is 0.129 nm in the FCC lattice, and the largest interstitial voids occur at the (1/2,0,0), (0,1/2,0), (0,0,1/2) etc. type positions. **(7 marks)**

3. A tin-bronze alloy consists of a substitutional solid solution of Sn atoms on a Cu FCC lattice, resulting in an alloy with lattice parameter 0.376 nm and a density of 8.772 g/m^3. Calculate the atomic concentration of tin present in the alloy. Molar mass for Sn is 118.71g while for Cu it is 63.546g.**(7 marks)**

Question IV: Diffusion

1. (a) What is diffusion flux? How is it related to the concentration gradient? **(3 marks)**
   (b) Will the diffusion of atoms occur from regions of low concentration to high concentration or the reverse is true. Why? **(2 marks)**
   (c) Does the rate of diffusion increase or decrease with increase in temperature? Explain using an equation. **(3 marks)**

2. The wear resistance of a steel gear is to be improved by hardening its surface. This can be accomplished by increasing the carbon content within an outer surface layer as a result of carbon diffusion into the steel. The carbon will be supplied from an external carbon-rich gaseous atmosphere at an elevated and constant temperature. The initial carbon content of the steel is 0.20 wt%, whereas the surface concentration is to be maintained at 1.00 wt%. In order for this treatment to be effective, a carbon content of 0.60 wt% must be established at a position 0.75 mm below the surface. Calculate the time consumed in heat treatment at temperatures of 900°C and 1050°C. Use following data for the diffusion of carbon in γ-iron: $D_0 = 5\times10^{-5}$ m^2/sec, E_{act} = 284 kJ/mol. **(12 marks)**. The error function values are 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: Dislocations, Slip and Grain Boundaries

1. Define the Burgers vector of a dislocation using an illustrative example. What is the difference between screw and edge dislocations? Explain using diagrams. **(5 marks)**

2. Explain how (i) dislocations, (ii) slip and (iii) ductility are related to each other? **(3 marks)**

3. Consider a single crystal rod of FCC nickel with a radius of 20 mm, oriented with the [100] direction parallel to the rod axis. **(3*4 = 12 marks)**
   a. Name the slip system involved in the plastic flow of nickel.
   b. How many of these slip systems are in a position to be activated at the same time when the load is applied parallel to this crystallographic direction?
   c. What is the Schmid factor for this slip system?
   d. Compute the minimum shear stress required to initiate slip in a pure and perfect single crystal in MPa if the crystal is loaded with an axial load of 50 kN.

Question VI: Mechanical Deformation

1. Explain the difference between: (a) yield strength and ultimate strength, (b) engineering stress and true stress. **(3 + 3 = 6 marks)**

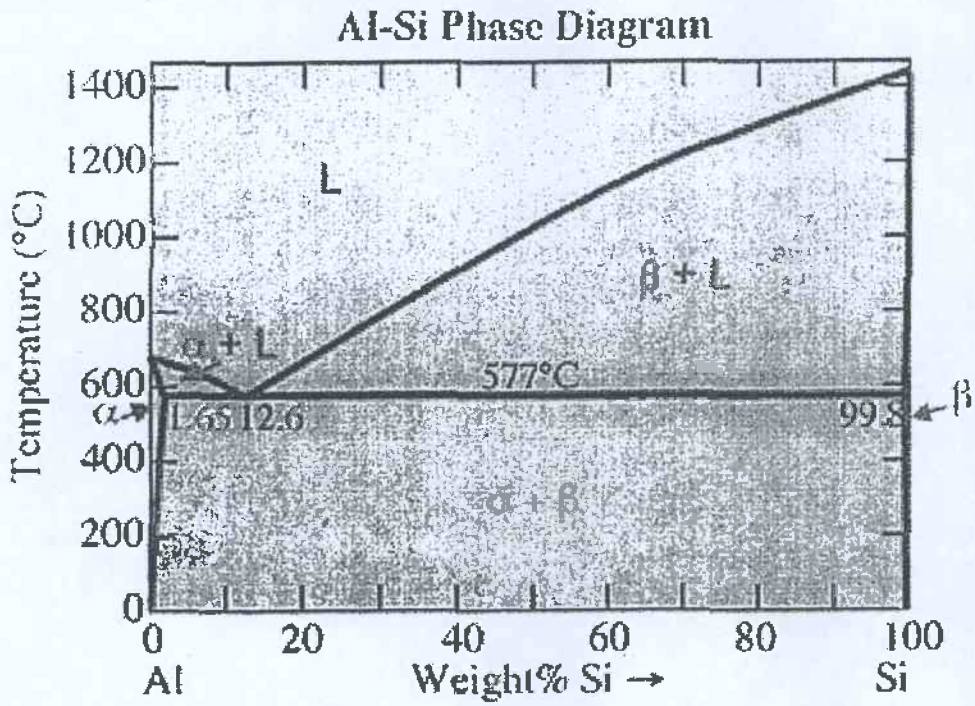
2. A 25 cm long rod with a diameter of 0.25 cm is loaded with a 2 kN weight. The material has a linear elastic-perfectly plastic stress-strain response. If the diameter decreases to 0.23 cm, *compute the following:*
   a. The final length of the rod assuming the volume is conserved. **(2 marks)**
   b. The true stress and true strain at this load. **(4 marks)**
   c. The engineering stress and strain at this load. **(4 marks)**
   d. The yield strength assuming 2.2% elongation at the yield point, and the elastic energy stored in the rod until the yield point. The Young's modulus is given as 210 GPa. **(4 marks)**

Question VII: X-ray Diffraction and Experimental Methods for Crystal Structure

1. Explain how you will use X-ray diffraction data to determine if a crystal is FCC or BCC utilizing the Bragg's law of diffraction. **(6 marks)**
2. The metal niobium has a BCC crystal structure. If the angle of diffraction for the (211) set of planes occurs at 75.99° (first order reflection) when monochromatic x-radiation having a wavelength of 0.1659 nm is used, compute:
   (a) The interplanar spacing for this set of planes,
   (b) The atomic radius for the niobium atom, and
   (c) The lowest angle peak in the x-ray diffraction of niobium, and the corresponding set of planes (hkl). **(4 + 4 + 6 = 14 marks)**

Question VIII: Phase Diagram

For the equilibrium phase diagram of Al- Si shown below, assume fully established phase equilibria at any given composition –temperature combination, as established during slow cooling.



1. For an alloy consisting of *50 wt% Al and 50 wt% Si determine the following:* **(2*4 = 8 marks)**
(a) The temperature at which the first solid would appear upon slow cooling from 1200°C.
(b) The composition of the first solid.
(c) The composition of the last liquid to solidify upon further cooling.
(d) The temperature at which the last liquid solidifies (ignoring super cooling effects).

2. *Al- Si alloys on the Al-rich side are* precipitation hardenable (age hardenable) up to a certain maximum composition. **(2*3 = 6 marks)**
(a) Determine this maximum composition from the phase diagram.
(b) Suggest a heat treating schedule (temperatures, times) that could be used to precipitation harden an alloy of your choice, beginning with the solutionizing heat treatment.
(c) Draw the microstructures in the solutionized, quenched and reheated states.

3) In the most general terms, a eutectic reaction such as the one shown in the Al-Si phase diagram can be written as: Liquid ↔ Solid 1 + Solid 2. Using a similar format, write down the reactions for the eutectoid, peritectic and monotectic reactions. **(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

$n = 1, 2, 3, \ldots$ $l = 0, 1, 2, \ldots n-1$ $m_l = 0, \pm1, \pm2, \pm3, \ldots \pm l$ $m_s = \pm 1/2$

$$\Delta x . \Delta p \geq \frac{h}{4\pi} \qquad \lambda = \frac{h}{mv} \qquad F = -\frac{\partial E}{\partial r}$$

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

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

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

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

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

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

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

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

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