National Exams December 2013

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

1. Briefly describe Bohr's model of atomic structure. What were its limitations, and how did the wave-mechanical model resolve some of these issues? **(6 marks)**

2. An extremely heavy element **ununpentium** has recently been confirmed.
   a. If you include this, how many elements are there in the periodic table?
   b. Recognizing that some of these are naturally occurring while some are man-made, provide at least one example of both element types?
   c. Is it true that lighter elements are naturally occurring, and heavier elements tend to be synthetic? Why/Why not?

   (2*3 = 6 marks)

3. A common way to describe the bonding energy curve for secondary bonding is the "6-12" potential, which states that
   $E = -\frac{A}{r^6} + \frac{B}{r^{12}};$
   where r is the interatomic spacing and the constants A , B are given as $A = 10.37 \times 10^{-78}$ J.m^6 and $A = 16.16 \times 10^{-135}$ J.m^{12}, for argon. Calculate the bond energy and bond length.
   (8 marks)

Question II: Crystal Defects

1. Define the following types of defects, with examples and diagrams **(2*5 = 10 marks)**
   a. Schottky defect
   b. Grain boundary
   c. Screw dislocation
   d. Stacking fault
   e. Partial dislocation

2. Small-diameter noble gas atoms, such as helium, can dissolve in a relatively open network structure of silicate glasses. The secondary bonding of helium in vitreous silica is represented by a heat of solution, ΔH_s, of -3.96 kJ/mol. The relationship between solubility, S, and the heat of solution follows the following relation: $S = S_0 e^{-\frac{\Delta H_s}{RT}}$, where S_0 is a constant, R is the gas constant, and T is the absolute temperature. If the solubility of helium in vitreous silica is 5.51×10^{23} atoms/(m^3-atm) at 25°C, calculate the solubility at 200°C. **(6 marks)**

3. Does the yield strength of an alloy increase or decrease when the grain-size is decreased? Explain why. **(4 marks)**

Question III: Crystal Structure

1. Define the following terms, using equations, diagrams and examples as applicable:

(a) Atomic packing factor

(b) Electronegativity

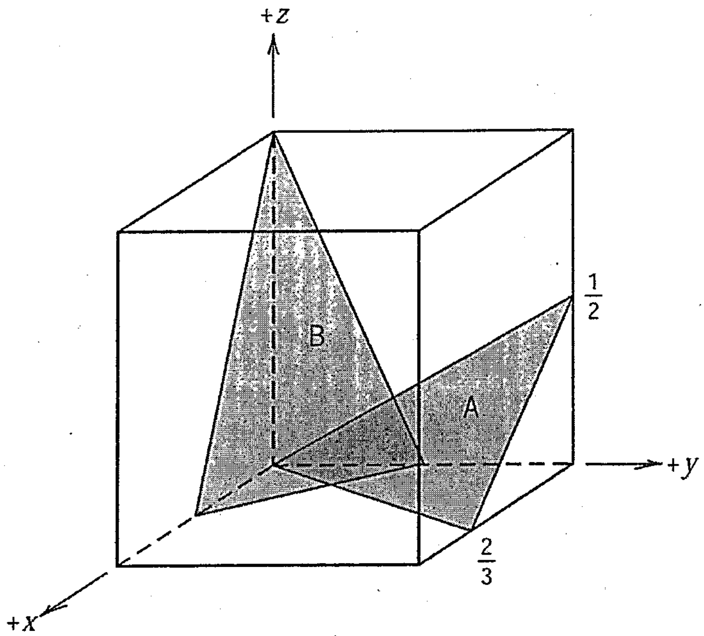
(c) Hexagonal close packed structure

(d) Miller Indices

(2*4 = 8 marks)

2. Derive the atomic packing factor for FCC. **(6 marks)**

3. Determine the Miller indices for the planes shown in the following unit cell. Clearly show your derivations. **(6 marks)**



Question IV: Structure and Chemical Bonding

1. Differentiate between primary and secondary bonding. Identify the type of chemical bonding in the following material systems:
   a. CsCl
   b. Inter-layer bonding in graphite
   c. Iron (Fe)
   d. Rubber
   e. Silica (SiO_2)

   (3 + 1*5 = 8 marks)

2. Sketch the the polymerization process for polyvinyl chloride (PVC) and calculate its reaction energy. The vinyl chloride molecule is C_2H_3Cl. **(6 marks)**

   The bond energies of different bonds are provided as: C-C bond =370 kJ/mol; C=C = 680 kJ/mol, C-H = 435 kJ/mol, C-O = 360 kJ/mol, C-Cl = 340 kJ/mol.

3. At room temperature, cobalt has the HCP crystal structure ($c/a = 1.623$) and an atomic radius of $r = 0.1253\ nm$. Calculate the theoretical density of Co. The molar mass of Co is 58.93 g/mol. **(6 marks)**

Question V: X-ray Diffraction and Microstructural Characterization

1. Briefly describe the principle and applications of the two electron microscopy techniques: (i) transmission electron microscopy (TEM), and (ii) scanning electron microscopy (SEM). **(6 marks)**

2. Nickel is face centered cubic and has an atomic radius of $r = 1.25 \times 10^{-10}\ m$.

   a. Calculate the 2θ values for the first three diffraction peaks that would be obtained in an X-ray diffraction run for a nickel powder sample using Cu-K_α radiation ($\lambda = 1.542 \times 10^{-10}\ m$). First, calculate the lattice parameter. Then write down possible planes and apply the reflection rules (see appendix). Now, calculate the d-values for these planes. Finally, calculate the 2θ values. **(10 marks)**
   b. How would this answer change if the nickel sample is a single crystal with the (100) plane parallel to the surface? **(4 marks)**

Question VI: Diffusion

A low carbon steel with 0.2% C is carburized in a hydrocarbon gas at 1000°C. The surface of the steel reaches a value of 1.0 %C very rapidly. Calculate the carbon content at a depth of 0.3 mm beneath the surface after 10 hours at this temperature. The diffusion coefficient for C in Fe is given as $D = 0.298 \times 10^{-6}$ cm^2/sec. Also calculate the time necessary to raise the carbon content at this location to 0.6%. The error function values are tabulated in the appendix.

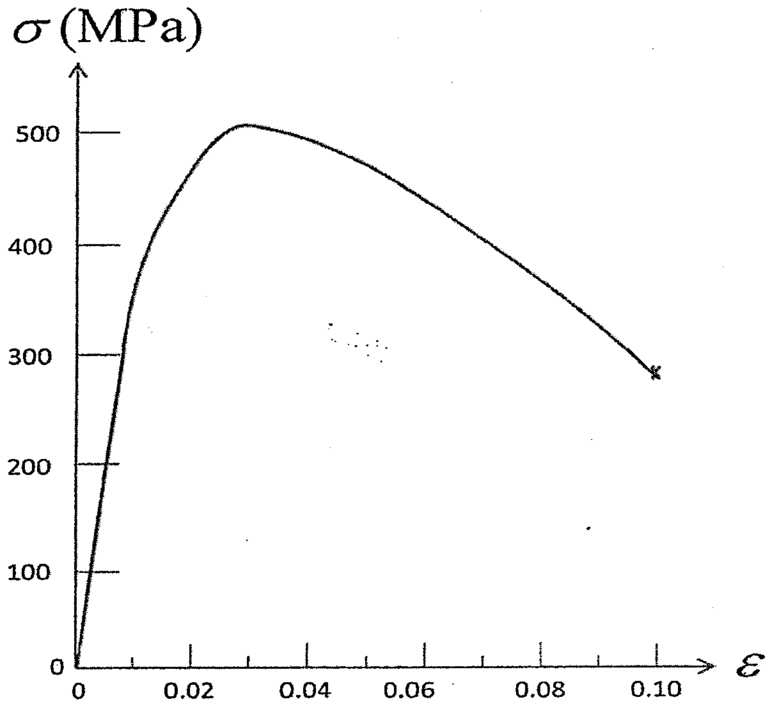
(20 marks)

Question VII: Mechanical Behaviour

1. What is the difference between ductility and fracture toughness? **(3 marks)**

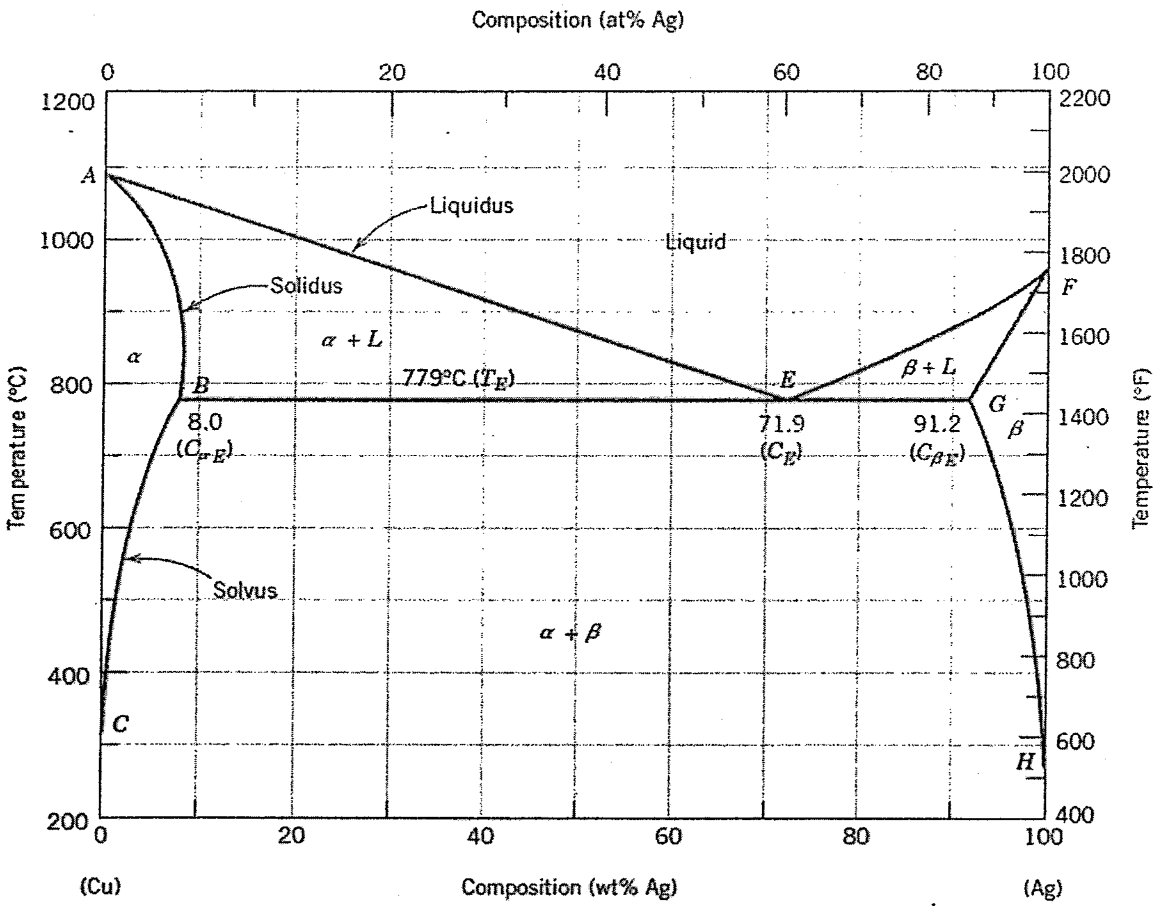
2. Draw the representative stress-strain curves for the following, identifying key points on the diagrams **(2*4 = 8 marks)**:
   a. a typical metallic alloy, e.g. steel
   b. brittle material, and
   c. linearly elastic-perfectly plastic material
   d. nonlinearly elastic material

3. For the stress-strain curve provided below, calculate the following properties **(1.5*6 = 9 marks)**:
   a. Yield strength, MPa
   b. Ultimate tensile strength, MPa
   c. Young's modulus of elasticity, GPa
   d. % elongation to failure
   e. Modulus of resilence (defined as the energy absorbed by the system in the elastic regime)
   f. Fracture toughness



Question VIII: Phase Diagram

For the binary eutectic phase diagram for copper-silver (Cu-Ag) shown below, answer the following questions: (**4 parts of 5 marks each=20 marks**)



1. For a 40 wt% Cu-60wt%Ag alloy at a temperature of 800°C, what phases are present in the system and what are their compositions?
2. At 700°C, what is the maximum solubility of: (a) Cu in Ag? (b) Ag in Cu?
3. Define eutectic reaction. Write the eutectic reaction for the Cu-Ag system.
4. Determine the relative mass fractions of the phases present in a 55wt%Ag-45wt%Cu alloy at 800°C.

Appendix: Equations and constants

Avogadro's number = 6.023×10^{23} molecules/mol   Universal gas constant (R) = 8.31 J/mol-K

Boltzmann's constant (k) = 1.38×10^{-23} J/atom-K = 8.62×10^{-5} eV/atom-K

1 MPa = 10^6 N/m^2 1 GPa = 10^9 N/m^2

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

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

$N_D = N \exp\left(-\frac{Q_D}{kT} \right)$ $N = \frac{\rho N_A}{A_{wt}}$; A_{wt} = atomic weight $T_K = T_C + 273$; $A = \pi r^2$; $V = \frac{4}{3}\pi R^3$

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

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

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

$\tau_R = \sigma.\cos\phi.\cos\lambda$ $\sigma = \sigma_0 + k.d^{-1/2}$ $\varepsilon = \frac{\Delta l}{l_0}$ $\sigma = \frac{F}{A_0}$ $\sigma = E\varepsilon$ $\tau = \frac{F}{A_0}$

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

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