National Exams May 2016

10-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.

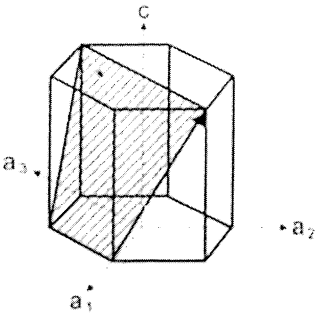
4. If a doubt exists as to the interpretation of any question, equation or data given, the candidate is urged to submit with the answer paper, a clear statement of any assumptions made.

Question I: Electron Structure and Bonding

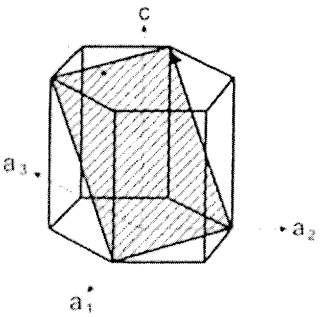
1. (**6 marks**) Explain, with an equation or an example, following principles for atomic structure of materials:
   a. Ground state energy
   b. Isotope (give example)
   c. Electronegativity
2. (**4 marks**) Differentiate between Bohr model and wave mechanical model for atomic structure. Draw schematic representations of both. Which one is more accurate and why?
3. (**8 marks**) Draw the periodic unit cells of following materials and identify bonding type in each of them: (i) NH_3, (ii) Cl_2, (iii) MgO, (iv) Diamond.
   (**2 marks**) Which materials amongst above are expected to have the highest and the lowest melting point, respectively?

Question II: Crystal Structure I

Cobalt has an HCP crystal structure at room temperature ($c/a = 1.623$). Its atomic radius is 0.1253 nm, and atomic weight is 58.933.



1. (**6 marks**) Calculate the theoretical density of Co.
2. (**4 marks**) Draw the following directions in its unit cell: $[10\bar{1}0], [1\bar{2}11]$
3. (**6 marks**) Calculate the planar densities of the planes shaded in right.
4. (**4 marks**) What are the linear densities for the directions in part 2 above?



Question III: Crystal Structure II

Barium titanate ($BaTiO_3$) has 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.

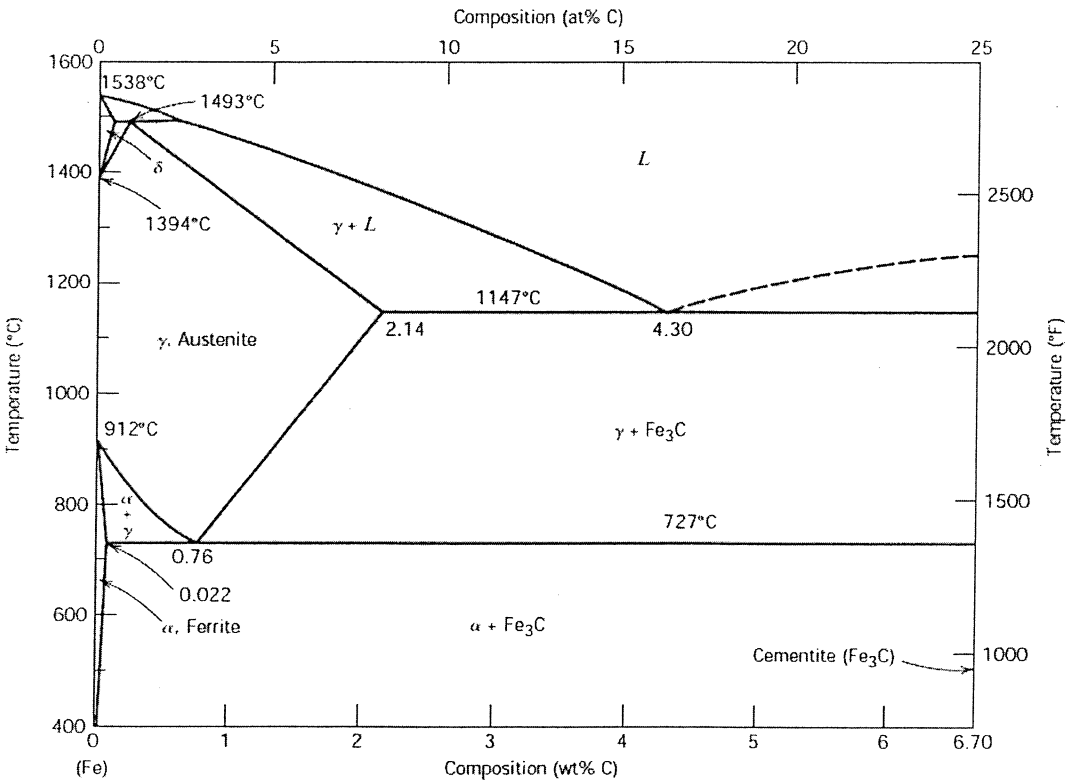
1. (**6 marks**) Draw the unit cell of $BaTiO_3$, showing the positions of all Ba^{2+}, Ti^{4+} and O^{2-} ions. Use different colors/symbols to clearly distinguish between different species.
2. (**8 marks**) The atomic weights for different species are given as: $A_{Ba} = 137$, $A_{Ti} = 48$, and $A_O = 16$. The density of $BaTiO_3$ is 6 g/cm^3. Calculate its lattice parameter.
3. (**6 marks**) An alternate way of drawing the unit cell of perovskite structure has Ba at the body-centred position of each cubic unit cell. What are the positions of the titanium and oxygen atoms in this representation of the unit cell? Draw this unit cell.

Question IV: Crystalline Imperfections

1. (**6 marks**) What are the four Hume-Rothery rules for metallic solid solutions? Apply these rules to address solubility of Cu into Ni, and conclude whether or not Cu is completely miscible in Ni.
2. (**8 marks**) A BCC iron crystal at room temperature has a lattice parameter of 0.2866 nm and a weight of 55.85 g/mol.
   (a) (**4 marks**) Calculate its theoretical density,
   (b) (**4 marks**) Calculate the number of vacancies needed for it to have a density of 7.874 g/cm^3.
3. (**6 marks**) Write down all the slip systems in for FCC and BCC crystal? For such crystals, write down the magnitude of the Burger's vector of an edge dislocation in terms of lattice parameter, a.

Question V: Phase Diagram

(**20 marks**) The binary eutectic phase diagram for iron-carbon (Fe-C) alloy system is shown below



1. (**6 marks**) Determine the temperatures and compositions of all invariant reactions in this system. Write down the phase reaction associated with each of the invariant reactions.
2. (**4 marks**) Determine the maximum solubility of carbon in α-ferrite and austenite phases.
3. (**4 marks**) For a 99.65 wt% Fe-0.35 wt% C alloy at a temperature just below 727°C, determine the fractions of phases present.
4. (**6 marks**) For a steel containing 1 wt% C, draw the equilibrium microstructures that would form at: (a) 1000°C, (b) 750°C, (c) 500°C.

Question VI: X-ray Diffraction

(**20 Marks**) An x-ray diffractometer recorder chart for an element which has either the BCC or the FCC crystal structure shows diffraction peaks at the following 2θ angles: 40°, 58°, 73°, 86.8°, 100.4°, and 114.7°. The first two sets of diffracting planes are {110} and {200} for the BCC crystal structure, and {111} and {200} for the FCC crystal structure. The wavelength of the incoming x-ray used was 0.154 nm. Determine the following:

1. (**5 marks**) The cubic structure of the element (i.e. whether it is FCC or BCC).
2. (**5 marks**) The lattice constant of the element.
3. (**6 marks**) The first two diffraction angles (2θ) corresponding to the other crystal structure (For example, if you obtained FCC in part 1, compute diffraction angles for BCC; and vice-versa).
4. (**4 marks**) Draw all the four planes in different cubic unit cells.

Question VII: Diffusion and Case Hardening

1. (**8 marks**) Suppose that interstitial atoms are found to move from one site to another at the rate of 5×10^8 jumps/s at 500°C and 8×10^8 jumps/s at 800°C. Calculate the activation energy in cal/mol for the process.

2. (**12 marks**) 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% C very rapidly. Calculate the carbon content at a depth of 0.2 mm beneath the surface after 8 hours at this temperature. The diffusion coefficient for carbon in iron at this temperature is 2.98×10^{-11} m^2/s.

VIII: Mechanical Deformation

1. (**8 marks**) Draw representative stress-strain plots for the following types of materials, and show important points on the graphs such as yield point, plastic strain, fracture, ultimate tensile strength **as applicable**:
   (a) Elastic – brittle, (b) Elastic – perfectly plastic,
   (c) Elastic – linear work hardening, (d) Hyperelastic (e.g. rubber).

2. (**12 marks**) For a 10-mm diameter rod of 3003-H14 aluminum alloy, the following material properties are given: $E = 70$ GPa, $\sigma_y = 145$ MPa, $\upsilon = 0.33$.
   (a) (**4 marks**) Calculate the diameter if this rod is subjected to a 6-kN tensile load.
   (b) (**4 marks**) Calculate the diameter if this rod is subjected to a 6-kN compressive load.
   (c) (**4 marks**) Calculate the plastic strain in the rod if it is subjected to a 15-kN tensile load.

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 1 eV = 1.6022×10^{-19} J

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

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

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

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

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

$J_x = -D\dfrac{\partial c}{\partial x}$ $\dfrac{\partial c_x}{\partial t} = D\dfrac{\partial^2 c_x}{\partial x^2}$ $\dfrac{C_s - C_x}{C_s - C_0} = erf\left(\dfrac{x}{2\sqrt{Dt}}\right)$ $D = D_0\exp\left(-\dfrac{Q_d}{RT}\right)$

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

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

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