National Exams December 2019

10-Met-A4, Structure of Materials

3 Hours Duration

NOTES:

1. Attempt any **five** questions out of **seven**. **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 1: Atomic Structure

1. (**2*4 = 8 marks**) Briefly explain, with appropriate examples and/or sketch, the following concepts regarding the atomic structure of materials:
   a. Four quantum numbers,
   b. Isotopes,
   c. Wave-mechanical atomic model,
   d. Radioactive decay.

2. (**2*3 = 6 marks**) Write down the complete electronic structures of following ions, with atomic numbers of the parent elements shown in the brackets:
   a. Fe^{3+} (Z = 26) b. Nb^{2+} (Z = 41) c. S^{2-} (Z = 16)

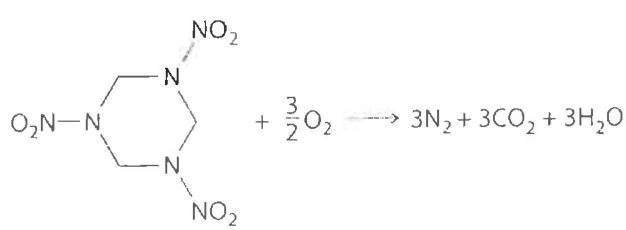
3. (**3 + 3 = 6 marks**) Assuming that the wave-particle duality holds, compare the wavelength of an electron moving at one fifth of the speed of light with that of a baseball with a mass of 0.142 kg traveling at 42.91 m/s. If the uncertainty associated with the measurement of their speeds is 1 percent, then what are the corresponding uncertainties in knowing their positions?

Question 2: Chemical Bonding

1. (**6 marks**) What is understood by polarity of covalent bonds? Which of the following molecules would one expect to have a non-polar covalent bond and why?
   (i) HCl (ii) F2 (iii) HF (iv) ClF.

2. (**3 + 3 = 6 marks**) Hydrogen bonds are formed in many compounds e.g., H_2O, HF, NH_3. Define hydrogen bonding and differentiate it with covalent bonding. Which one of these compounds will have the highest boiling point and why?

3. (**6 + 2 = 8 marks**) The compound RDX (Research Development Explosive) is a powerful explosive commonly used by the military. When detonated, it produces gaseous products and heat according to the following reaction. Use the approximate bond energies tabulated below to estimate the ΔH_{rxn} per mole of RDX. Is the reaction exothermic or endothermic?



RDX

Bond	H-H	C-C	H-C	O-O	O-H	C-N	N-N	N-O	N=O	O=O	C=O
ΔH (KJ/mol)	432	346	411	142	459	305	167	201	607	494	799

Question 3: Crystal Structure

1. **(6 marks)** Draw the following crystal directions and planes in simple cubic and hexagonal cubic unit cells:
   a. $[1\bar{2}1]$ b. (232) c. $(1\bar{2}10)$

2. **(4 marks)** Many oxides such as $CaTiO_3$ assume the perovskite crystal structure. Draw the full crystal structure of $CaTiO_3$, clearly identifying different ions and their positions in your sketch.

3. **(10 marks)**

   a. **(2 marks)** Calculate the volume of an HCP unit cell in terms of its a and c lattice parameters.

   b. **(2 marks)** Now provide an expression for this volume in terms of the atomic radius, R, and the c lattice parameter.

   c. **(3 marks)** Compute the atomic packing factor for HCP crystal with $c = 1.633\ a$.

   d. **(3 marks)** Rhenium has an HCP crystal structure, an atomic radius of 0.137 nm, and a c/a ratio of 1.615. Compute the volume of the unit cell for Re.

Question 4: Point Defects in Crystalline Solids

1. **(6 marks)** 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.

2. **(2 + 2 + 2 = 6 marks)** Explain why real crystals will always contain point defects. What is the effect of temperature on equilibrium density of point defects? If their equilibrium density at two different temperatures T_1 and T_2 is denoted by ρ_1 and ρ_2, respectively, then derive the relation for ρ_1/ρ_2.

3. **(4 + 4 = 8 marks)** Calculate the concentration of vacancies in copper at 25°C. What temperature will be needed to heat treat copper such that the concentration of vacancies produced will be 1000 times more than the equilibrium concentration of vacancies at room temperature? Assume that 83,680 J are required to produce a mole of vacancies in copper.

Question 5: Microstructural Characterization

1. **(20 marks)** Nickel is face centered cubic and has an atomic radius of $R = 0.125\ nm$.

a. **(12 marks)** 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 ($\lambda = 0.1542\ nm$). First, calculate the lattice parameter. Then write down possible planes and apply the appropriate reflection rules. Now, calculate the interplanar spacing for these planes. Finally, calculate the 2θ values.

b. **(4 marks)** How would this answer change if the nickel sample is a single crystal with the (100) plane parallel to the surface?

c. **(4 marks)** Using XRD, how would you determine if a metal has FCC or BCC crystal structure?

Question 6: Dislocations and Grain Boundaries

1. **(10 marks)**
   a. **(4 marks)** Explain how (i) dislocations, (ii) slip, (iii) yield strength, and (iv) ductility are related to each other.

   b. **(6 marks)** Explain what is meant by cross slip of a dislocation. What material characterization method can you use to confirm the presence of a cross-slip in a deformed crystal? What role does this phenomenon play in the plasticity behavior of metallic systems?

2. **(10 marks)** Consider a single crystal of BCC iron oriented such that a tensile stress is applied along a [010] direction.

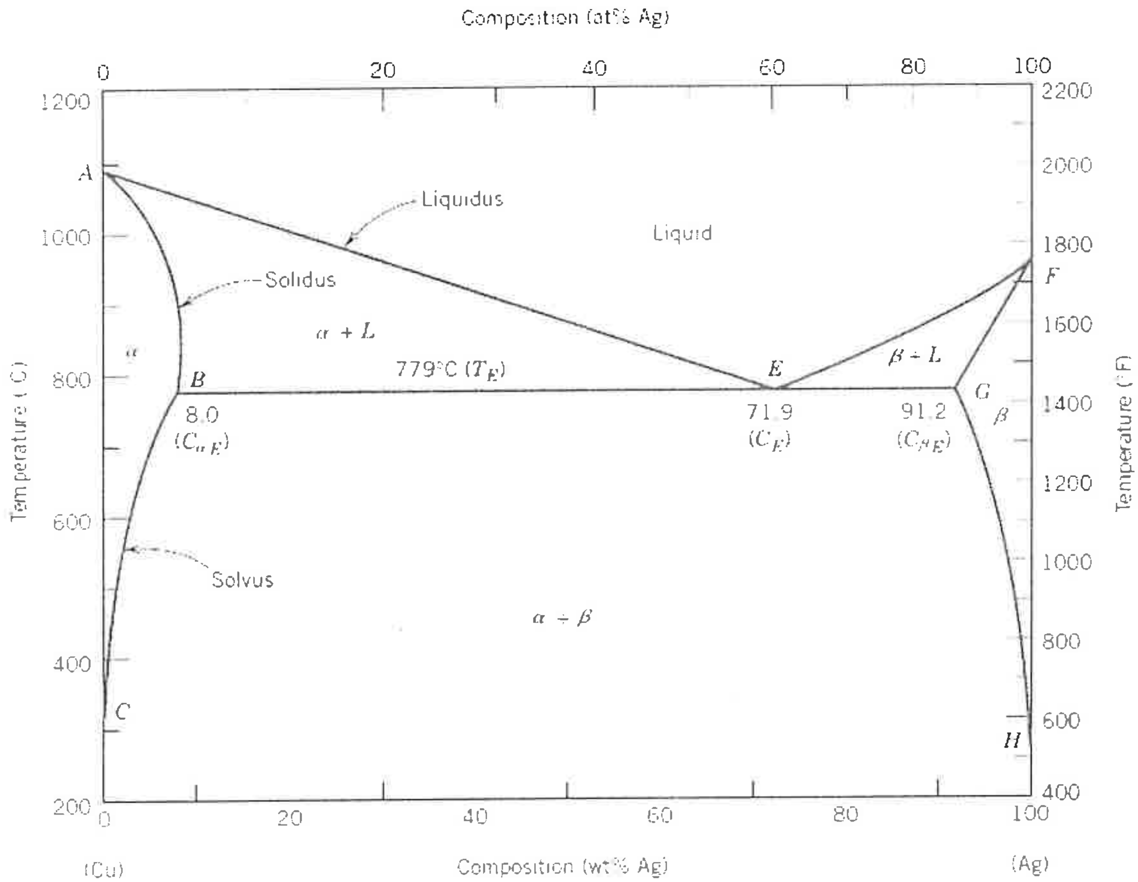
   a. **(3 marks)** Compute the resolved shear stress along a (110) plane and in a [111] direction when a tensile stress of 52 MPa is applied.

   b. **(3 marks)** If slip occurs on a (110) plane and in a [111] direction, and the critical resolved shear stress is 30 MPa, calculate the magnitude of the applied tensile stress necessary to initiate yielding.

   c. **(4 marks)** Write down possible slip systems for BCC iron and FCC copper by listing the different combinations of slip planes and slip directions.

Question 7: Phase Diagram

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



1. (**4 marks**) 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. (**4 marks**) At 700°C, what is the maximum solubility of: (a) Cu in Ag? (b) Ag in Cu?

3. (**4 marks**) Define eutectic reaction. Write eutectic reaction for the Cu-Ag system, indicating the compositions of the phases involved and the temperature at which this reaction occurs.

4. (**4 marks**) Determine the relative mass fractions of the phases present in a 55wt%Ag-45wt%Cu alloy at 800°C.

5. (**4 marks**) If a 20wt%Ag-80wt%Cu alloy is cooled from 1100°C to room temperature, schematically draw the microstructure at different temperatures, depicting solidification, precipitation and subsequent microstructural development

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 eV = 1.6022×10^{-19} J

Planck's constant, $h = 6.63 \times 10^{-34}$ J.s ;   Electron mass, $m_e = 9.11 \times 10^{-31}$ kg;   Speed of light, $c = 3\times10^{8}$ m/s

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

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

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

$E = h\nu$ $\nu\lambda = c$ $\lambda = \dfrac{h}{mv}$ $\Delta x.\Delta p \ge \dfrac{h}{4\pi}$

$N_D = N\exp\left(-\dfrac{Q_D}{kT}\right)$ $N = \dfrac{\rho N_A}{A_{wt}}$; 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