National Exams May 2014

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, 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 theoretical principles for atomic structure of materials:
   a. Hiesenberg uncertainty principle
   b. Aufbau principle

2. **(4 marks)** Write down electronic configuration Iron (Fe), with atomic number $Z = 26$; and Titanium (Ti) with $Z = 22$, in terms of quantum numbers.

3. **(10 marks)** The net potential energy, E_N, between two adjacent ions of opposite charge (e.g. K^+ and Cl^-) can be expressed as the sum of an attractive energy and a repulsive energy,

$$E_N = -\frac{1.436}{a} + \frac{5.86\times10^{-6}}{a^9}$$

   In this expression the energy is expressed in eV and 'a' is the inter-ionic distance in nm. Calculate the bonding energy E_0 and schematically draw the E_N versus 'a' curve. In the plot, identify equilibrium value of inter-ionic distance and E_0.

Question II: Crystal Structure and Point Defects

1. **(8 marks)** Draw the following planes and directions (use separate drawings).
   (a) Planes in cubic unit cells: $(1\bar{1}0)$, $(2\bar{1}1)$
   (b) Directions in hexagonal close packed (hcp) unit cells: $[\bar{1}010],[11\bar{2}0]$

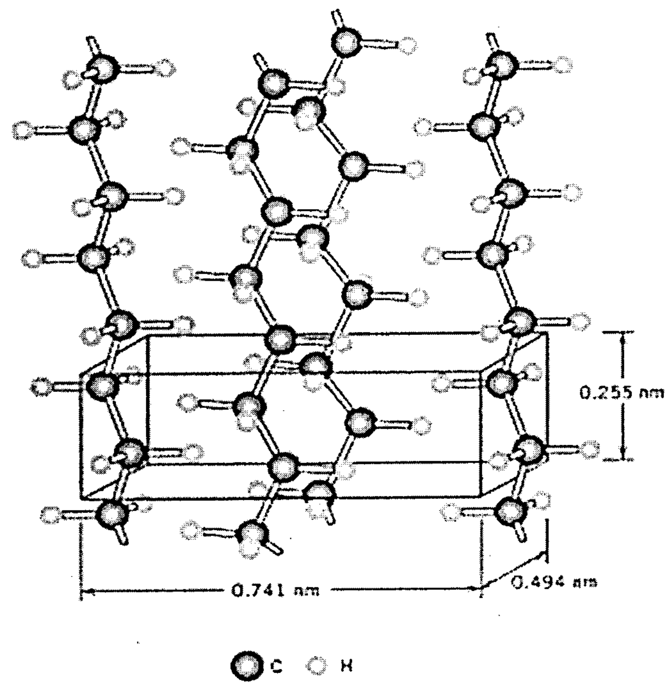
2. **(6 marks)** The density of vanadium (Z=23) is 5.8 g/cm^3. Determine whether it has a face centered cubic or body centered cubic crystal structure. It is provided that the unit cell length is 0.303 nm and the molar mass is 50.94 g/mol.

1. **(6 marks)** Explain the factors that govern solubility of one element in another. Using the data provided below, predict the relative degree of solubility of zinc and lead in copper.

Element	Atom radius (nm)	Crystal structure	Electronegativity	Valence
Copper	0.128	FCC	1.8	+2
Zinc	0.133	HCP	1.7	+2
Lead	0.175	FCC	1.6	+2, +4

Question III: Polymer Structure

1. **(6 marks)** Thermoplastic polymers exhibit stress relaxation where under a constant strain, the stress level decreases with time, given as $\sigma = \sigma_0 \exp\left(-\frac{t}{\tau}\right)$, where σ_0 denotes initial stress, and τ represents the relaxation time.
   A band of such polymer is used to hold together a bundle of steel rods for up to one year. If the stress on the band is less than 10 MPa, the band will not hold the rods tightly. Determine the initial stress that must be applied to the band when it is slipped over the steel. A series of tests showed that an initial stress of 7 MPa decreased to 6.8 MPa after six weeks.
2. **(4 marks)** Differentiate between thermosetting and thermoplastic polymers in terms of their structure and properties, especially the effect of temperature.
3. **(10 marks)** Polyethylene has an orthorhombic unit cell, as shown in figure. It is equivalent of two ethylene repeat units contained within each unit cell.
   a. **(6 marks)** Assuming a fully crystalline nature, compute its density in g/cm^3. Atomic weights for carbon and hydrogen are given as 12.01 g/mol and 1.008 g/mol.
   b. **(4 marks)** If a branched polyethylene has a density of 0.925 g/cm^3, calculate its percent crystallinity. The density for the totally amorphous material is 0.870 g/cm^3.



Question IV: Diffusion

1. **(6 marks)** A plate of iron is exposed to a carburizing atmosphere on one side and a decarburizing atmosphere on the other side at 700°C. Assuming steady-state diffusion, calculate the diffusion flux of carbon through the plate if the concentrations of carbon at positions of 5 and 10 mm beneath the carburizing surface are 1.2 and 0.8 kg/m^3, respectively. Assume a diffusion coefficient of 3×10^{-11} m^2/s.

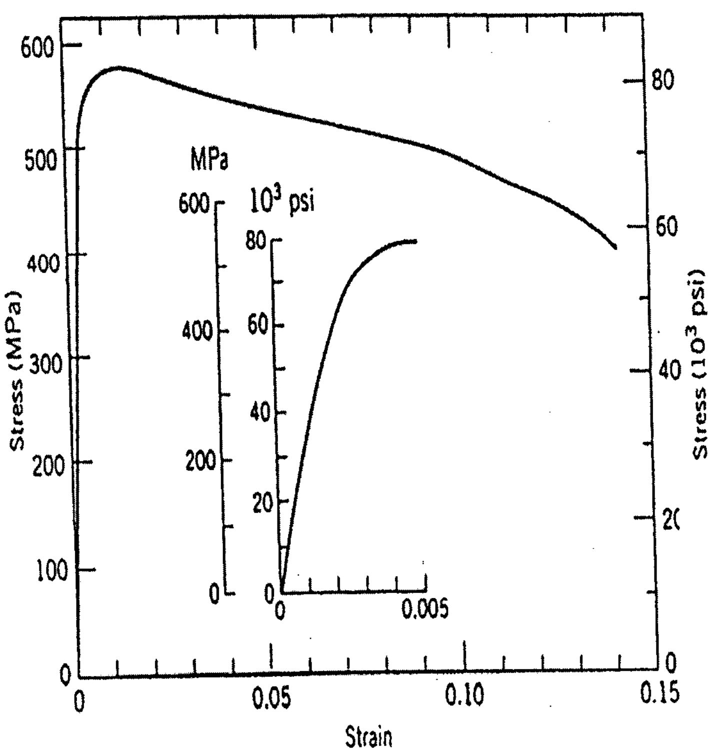
2. **(14 marks)** A steel plate, with an initial uniform carbon concentration of 0.25 wt%, is treated under carburising environment at the surface with a carbon concentration of 1.20 wt%. How long will it take to achieve a carbon content t of 0.80 wt% at a position 0.5 mm below the surface? The diffusion coefficient for carbon in iron at this temperature is 1.6×10^{-11} m^2/s.

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

1. **(20 Marks)** One promising candidate for Lithium Ion batteries is $LiMnPO_4$ which has a primitive orthorhombic crystal structure with lattice parameters a = 0.611 nm, b = 1.04 nm, and c = 0.475 nm. By computing the 2θ diffraction angle of the first four diffraction peaks, sketch a schematic diagram of the expected powder diffraction pattern for LiMnPO4 if it was characterized using Co K_α radiation (λ= 0.179 nm). Note that primitive crystal structures will yield diffraction peaks for each unique interplanar spacing.

VI: Mechanical Deformation

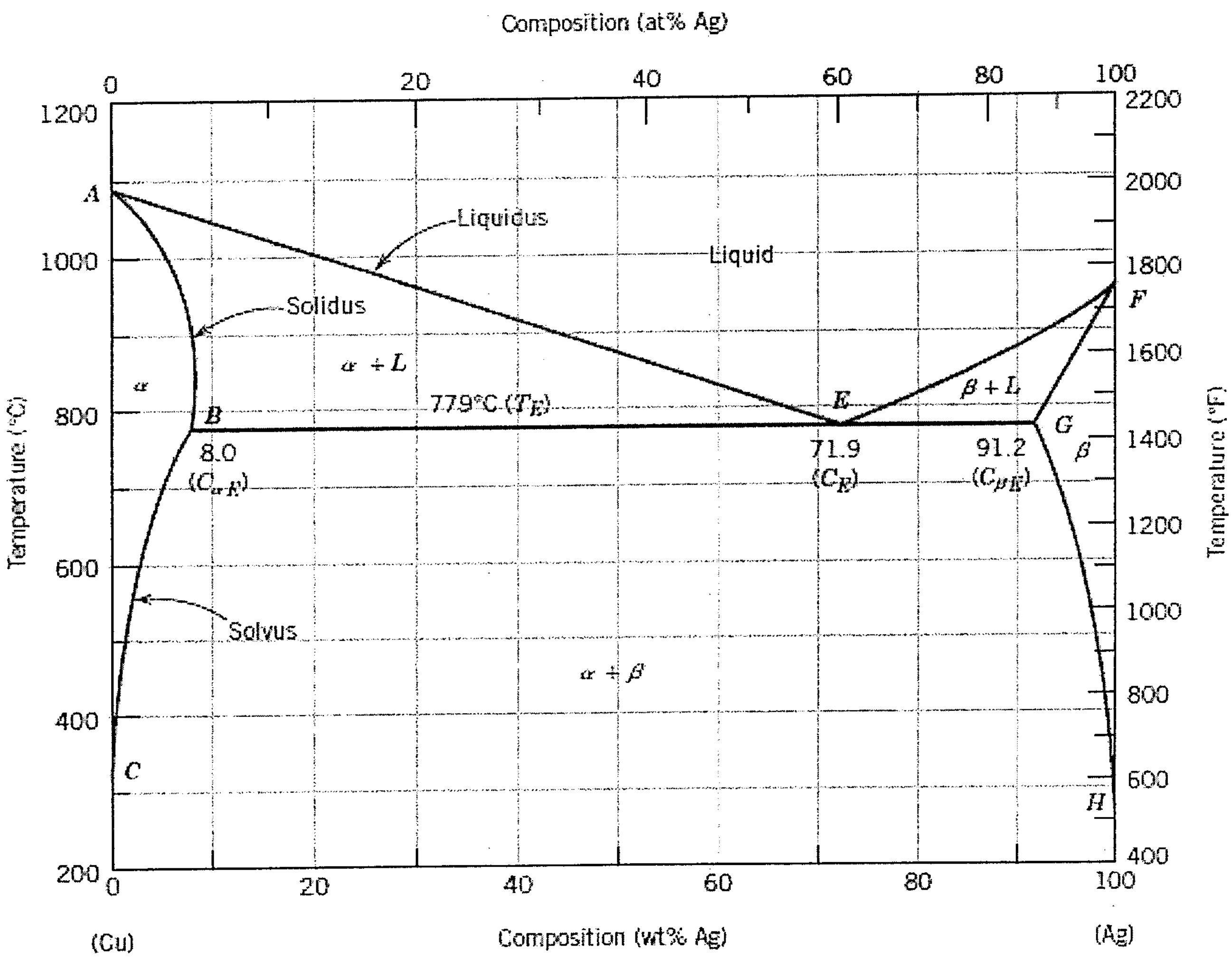
1. **(5 marks)** What is meant by critical resolved shear stress, τ_{crss}? Under what condition, is its maximum achieved? Relate yield stress, σ_y, to τ_{crss}.
2. **(5 marks)** Very briefly, explain three strengthening mechanisms for crystalline solids.
3. **(10 marks)** For the tensile stress-strain response shown below, determine:
   a. **(2 marks)** Young's modulus in GPa.
   b. **(2 marks)** Yield strength in MPa, based on a 0.2% strain offset.
   c. **(3 marks)** Determine the magnitude of the load required to produce a 2.5 μm reduction in diameter for a rod of this material with an initial diameter of 10 mm, if the deformation is entirely elastic. The Poisson's ratio is given as 0.34.
   d. **(3 marks)** If the material was loaded beyond the maximum stress point in the stress-strain curve, to a stress level of 500 MPa, and then unloaded fully, determine the amount of permanent residual strain in the material.



Question VII: Phase Diagram

The binary phase diagram for copper-silver (Cu-Ag) is shown below: **(5 parts of 4 marks each=20 marks)**

1. At 600°C, what is the maximum solubility of (a) Cu in Ag, (b) Ag in Cu.
2. What are the phases present at 20% Ag content and a temperature of 800°C? Determine their relative fractions.
3. For an alloy with 25% Ag content at 775°C, determine the mass fractions of α and β phases.
4. Define eutectic reaction. Write the eutectic reaction for the Cu-Ag system.
5. Briefly explain why, upon solidification, an alloy of eutectic composition forms a microstructure consisting of alternating layers of the two solid phases.



Question VIII: Dislocations and Grain Boundaries

1. **(10 marks)** Differentiate between the following with sketches and examples, as applicable
   a. **(6 marks)** Full dislocation and partial dislocation. Give examples of materials where each can be found, and write down the Burgers vectors for these dislocations.
   b. **(4 marks)** Tilt boundary and twist boundary

2. **(10 marks)** The relation between grain size (*d*) and yield strength of a metallic alloy can be expressed as $\sigma_y = \sigma_i + k_y d^{-\frac{1}{2}}$, where $\sigma_i = 3\ \text{MPa}$ is the friction stress, and $k_y = 0.5\ \text{MPa.}\,\text{m}^{\frac{1}{2}}$ is a constant. As received sample of this alloy has an average grain size of 4 μm. After annealing, the grain size increases to 103.82 μm.
   a. **(5 marks)** Calculate percentage decrease in yield strength of the alloy due to annealing.
   b. **(5 marks)** The grain growth during this process follows the relation $d^n - d_0^n = Kt$, where d_0 and d represent initial and final grain sizes for the process, t is time, and $n = 4$ and $K = 4.4$ $\mu\text{m}^n\text{s}^{-1}$ are constants. Determine the time taken by annealing process.

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

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

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

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

$a = 2R$ $a = 2\sqrt{2}R$ $a = \dfrac{4}{\sqrt{3}}R$ $APF = \dfrac{V_s}{V_c}$ $\rho = \dfrac{n.A_{wt}}{V_c.N_A}$ % crystallinity $= \dfrac{\rho_c(\rho_s - \rho_a)}{\rho_s(\rho_c - \rho_a)}$

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

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

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

$\dfrac{C_s - C_x}{C_s - C_0} = erf\left(\dfrac{x}{2\sqrt{Dt}}\right)$

$D = D_0\exp\left(-\dfrac{Q_d}{RT}\right)$

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