# National Exams May 2012

# 98-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.

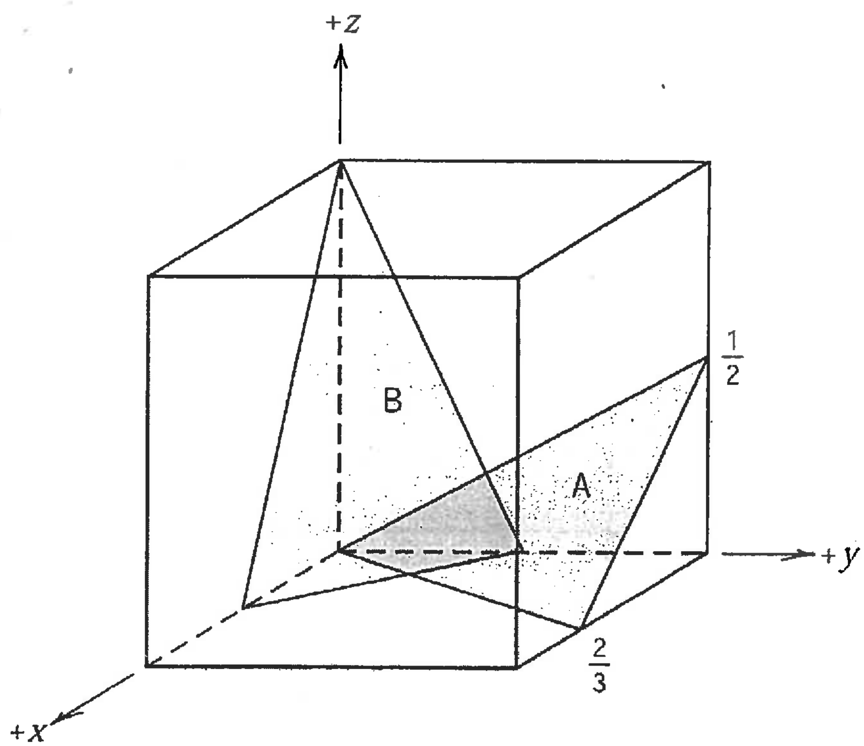
4. If a doubt exists as to the interpretation of any question, the candidate is urged to submit with the answer paper, a clear statement of any assumptions made.

## Question I: Electron Structure and Bonding

1. State the following two principles: (a) Pauli's exclusion principle, (b) Heisenberg uncertainty principle. **(3+3=6 marks)**
2. Suppose the net potential energy between two atoms is given by: $E = -\frac{A}{r^m} + \frac{B}{r^n}$, where $r$ is the interatomic spacing and $A$ and $B$ are constants. Derive an expression for the equilibrium interatomic spacing and the maximum binding energy. **(10 marks)**
3. Calculate the energy of a photon emitted when an electron in a hydrogen atom undergoes a transition from $n = 3$ to $n = 2$ state. Is the energy absorbed or emitted? **(4 marks)**

## Question II: Crystal Structure

1. Show that the atomic packing factor for BCC crystal structure is 0.68. **(8 marks)**
2. Determine the Miller indices for the planes shown in the following unit cell. Clearly show your derivations. **(6 marks)**




3. Calculate the theoretical volume change if a pure metal undergoes a polymorphic transformation in from BCC to FCC crystal structure. Assume the hard-sphere atomic model and that there is no change in atomic volume before and after the transformation. **(6 marks)**

## Question III: Point Defects in Crystals

1. 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 $\rho_1$ and $\rho_2$, respectively, then determine $\rho_1/\rho_2$ if $T_1/T_2=4$. **(6 marks)**
2. What is the difference between interstitial and substitutional impurity defects? Explain using a schematic representation and provide at least one example of each. **(6 marks)**
3. 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. **(8 marks)**

| 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 IV: X-ray Diffraction

1. Iridium has an FCC crystal structure. If the angle of diffraction for the (220) set of planes occurs at 69.22° (first order reflection) when monochromatic x-radiation having a wavelength of 0.0711 nm is used, compute (a) the interplanar spacing for this set of planes, and (b) the atomic radius for the iridium atom. **(8 marks)**
2. 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 $2\theta$ 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:
   a. The cubic structure of the element **(4 marks)**
   b. The lattice constant of the element **(4 marks)**
   c. The first two diffraction angles ($2\theta$) corresponding to the other crystal structure **(4 marks)**

## Question V: Diffusion

1. Briefly describe Fick's two laws for atomic diffusion. What are the parameters that affect the rate of diffusion? Explain how they affect the rate. **(6 marks)**
2. Consider the gas carburising of a gear of 1020 steel at 927°C. Assume that the carbon content at the surface is 0.90% and that the steel has a nominal carbon content of 0.20%. The diffusion coefficient at 927°C is equal to $1.28 \times 10^{-11}$ $m^2/s$.
   a. Calculate the time in seconds necessary to increase the carbon content to 0.52% at 0.500 mm below the surface. **(7 marks)**
   b. If the carburising is performed for 2.4 hours, calculate the carbon content at 0.50 mm beneath the gear surface. **(7 marks)**

You might need the error function values provided in the following table

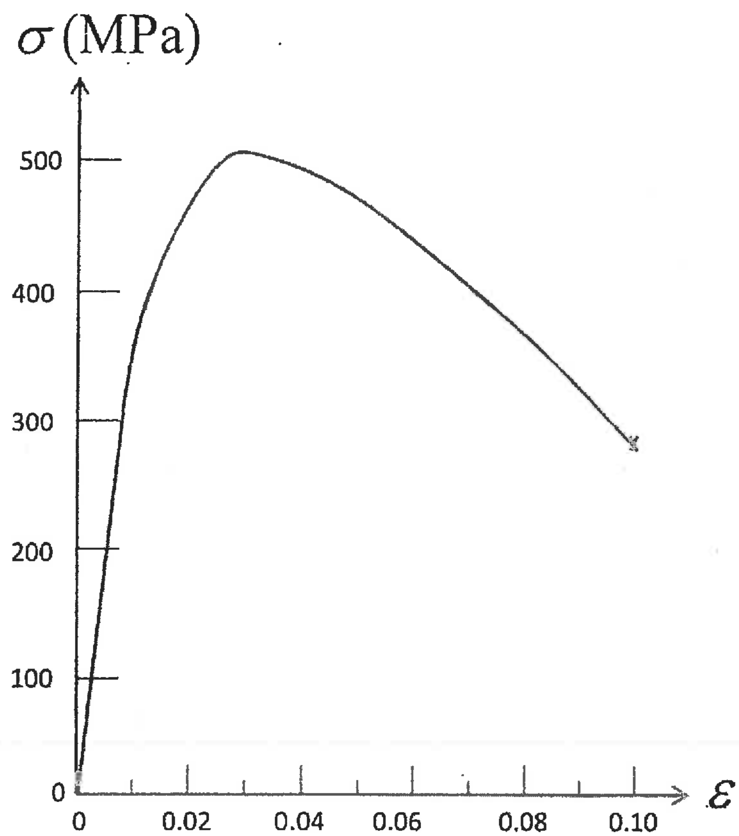
| Z | Erf(Z) |
|---|---|
| 0.50 | 0.52050 |
| 0.55 | 0.56332 |
| 0.60 | 0.60386 |
| 0.65 | 0.64203 |
| 0.70 | 0.67780 |
| 0.75 | 0.71116 |
| 0.80 | 0.74210 |
| 0.85 | 0.77067 |
| 0.90 | 0.79691 |

## Question VI: Dislocations, Slip and Grain Boundaries

1. What is the difference between: (a) screw and edge dislocations? (b) tilt and twist grain boundaries? Explain with schematics. **(8 marks)**
2. During strain hardening, the density of dislocations in the material rises. The critical resolved shear stress (CRSS) can be expressed as a function of dislocation density by $\tau_{crss} = \tau_0 + \alpha G b \sqrt{\rho}$ where $\tau_0$ is the intrinsic strength, $\alpha$ is a material constant, $G$ is the shear modulus, $b$ is the Burgers vector, and $\rho$ is the dislocation density per unit area. For a copper polycrystal, determine the following:
   a. What are the slip planes and slip directions? How many slip systems are present in the material? **(4 marks)**
   b. Determine the Burgers vector of an edge dislocation in the slip plane and its magnitude if the lattice constant of copper is 3.615 Å. **(3 marks)**
   c. If CRSS is equal to 2.1 MPa at a dislocation density of $10^5$ /mm$^2$, determine the value of $\tau_{crss}$ at a dislocation density of $10^7$ /mm$^2$. The shear modulus is 48 GPa and $\alpha$ =0.2. **(5 marks)**

## Question VII: Mechanical Deformation

1. Briefly describe four strengthening mechanisms for crystalline solids that lead to increase in yield strength or hardness of the material. **(4 marks)**
2. Tensile stress-strain curve for an aluminum 2024-T81 alloy specimen is shown below




For the given stress-stress curve, answer the following:

a. Determine the Young's modulus of elasticity, the yield strength at a 0.02% strain offset, the ultimate tensile strength, and % elongation at failure. **(4 marks)**.

b. Consider a cylindrical specimen of the alloy 10.0 mm in diameter and 75 mm long that is pulled in tension. Determine its elongation when a load of 20,000 N is applied. **(3 marks)**

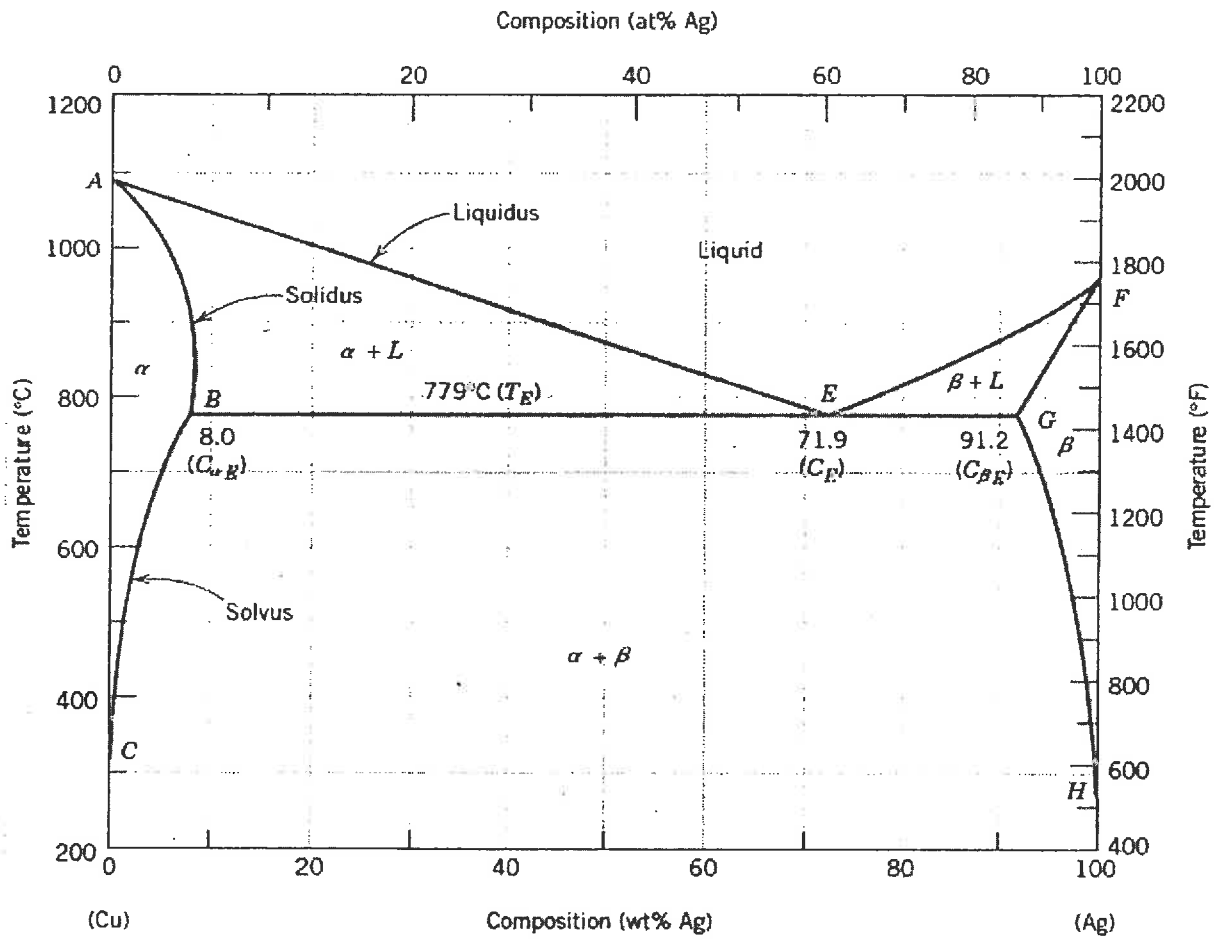
c. Calculate the maximum load that can be sustained by a cylindrical specimen having an original diameter of 12.8 mm. **(3 marks)**

d. The modulus of resilience for a specimen subjected to a uniaxial tension test is defined as the area under stress-strain curve upto yield point, i.e. $U_r = \int_0^{\varepsilon_y} \sigma \, d\varepsilon$. Derive an expression for $U_r$ in terms of Young's modulus, $E$, and the yield stress $\sigma_y$ and compute it for the given brass alloy. **(3 marks)**

e. Compare $U_r$ for the given Al alloy with brass that has Young's modulus of 97 GPa and yield strength of 250 MPa. What conclusion can you draw from the comparison? **(3 marks)**

## 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 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 $6.023 \times 10^{23}$ molecules/mol

Boltzmann's constant ($k$) $1.38 \times 10^{-23}$ J/atom-K = $8.62 \times 10^{-5}$ 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$^2$

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

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

$$N_D = N\exp\left(-\frac{Q_D}{kT}\right) \qquad N = \frac{\rho N_A}{A}$$

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

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

$$\tau_R = \sigma.\cos\phi.\cos\lambda$$

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

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

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

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

$$\sigma = \sigma_0 + k.d^{-1/2}$$