National Exams May 2008

Structure of Materials

3 Hours Duration

NOTES

1 If 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

2 Candidates may use one of two calculators, the Casio or Sharp approved models This is a Closed Book exam All equations, constants and diagrams are given in the appendix

3 **Any five** questions constitute a complete paper **Only the first five questions** as they appear in your answer book will be marked

4 All questions are of equal value

Question I Electron Structure and Bonding

1 Give the electron configurations for Ni^{2+} and S The atomic number of Ni is 28 and the atomic number of sulphur is 16 **(4 marks)**

2 Derive an expression for the equilibrium interatomic spacing if the net potential energy between two atoms is given by $E_N = -\frac{A}{r} + \frac{B}{r^n}$ where r is the interatomic spacing and A and B are system constants **(8 marks)**

3 Sketch the net force as a function of the interatomic spacing for two atoms indicating the equilibrium spacing r_0 and showing how the stiffness is related to the curve **(4 marks)**

4 Consider the hypothetical case of two materials having the same crystal structure and bond energy but in one case the bonds are metallic and in the other case the bonds are covalent *Briefly* explain how the bond type would be expected to affect the mechanical properties **(4 marks)**

Question II Metallic Crystals

An iron bar (of diameter 10 mm and length 100 mm) is galvanized with a thin coating of Zn At room temperature Fe has the BCC crystal structure while Zn has the HCP crystal structure (with c/a = 1 86) The molar mass of Fe is A_{Fe} = 55 85 g/mol and the molar mass of Zn is A_{Zn} = 65 41 g/mol

1 Estimate the lattice parameter of Fe if the bar weighs 61 78 g before galvanization **(10 marks)**

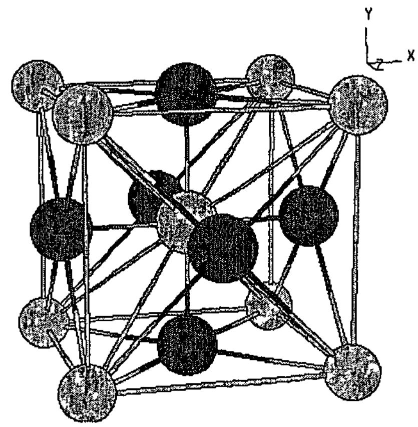
2 How many Zn atoms are in the coating if the average thickness is 50 μm? Assume an atomic radius for Zn of 0 133nm **(10 marks)**

Question III X-ray Diffraction

Li ion batteries having $LiCoO_2$ cathodes are widely used to power laptops and cell phones Considerable research has been conducted in the last decade to find next generation Li ion cathode materials One promising candidate 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 The interplanar spacing d for an orthorhombic crystal structure can be expressed as

$$\frac{1}{d^2} = \frac{1}{a^2}h^2 + \frac{1}{b^2}k^2 + \frac{1}{c^2}l^2$$

Sketch a schematic diagram of the expected powder diffraction pattern for $LiMnPO_4$ giving numerical values for the 2θ diffraction angle of the first four diffraction peaks (i e those planes corresponding to the four smallest 2θ values) if the $LiMnPO_4$ was characterized using Co K_α radiation (λ = 0 179 nm) **(20 marks)**



Question IV Ceramic Crystals

Barium titanate ($BaTiO_3$) has the perovskite crystal structure shown right Barium cations are located at the unit cell corners (r_{Ba} = 0 136 nm) oxygen anions are located on the unit cell faces (r_O = 0 140 nm) and a titanium cation is located at the unit cell centre (r_{Ti} = 0 061 nm) The molar masses of the constituent elements are A_{Ba} = 137 33 g/mol A_{Ti} = 47 87 g/mol and A_O = 16 00 g/mol you may assume a lattice parameter for $BaTiO_3$ of a = 0 39 nm

1 Calculate the atomic packing factor of $BaTiO_3$ **(6 marks)**

2 Calculate the theoretical density of BaTiO3 **(6 marks)**

3 Sketch the ion positions and determine the cation planar density on the (100) (110) and (111) planes **(6 marks)**

4 Determine the anion planar densities on the (100) and (200) planes **(2 marks)**

Question V Point Defects

1 Calculate the fraction of (1) vacant lattice sites and (2) self interstitial sites for nickel at its melting temperature of 1728 K Assume an energy of 0 7 eV/atom for vacancy formation and an energy of 1 4 eV/atom for self interstitial formation **(10 marks)**

2 Briefly explain the different vacancy and self interstitial concentrations **(4 marks)**

3 Ni is face centered cubic Calculate the size of the octahedral interstitial sites for Ni in terms of the lattice parameter a **(6 marks)**

Question VI Polymer Structures

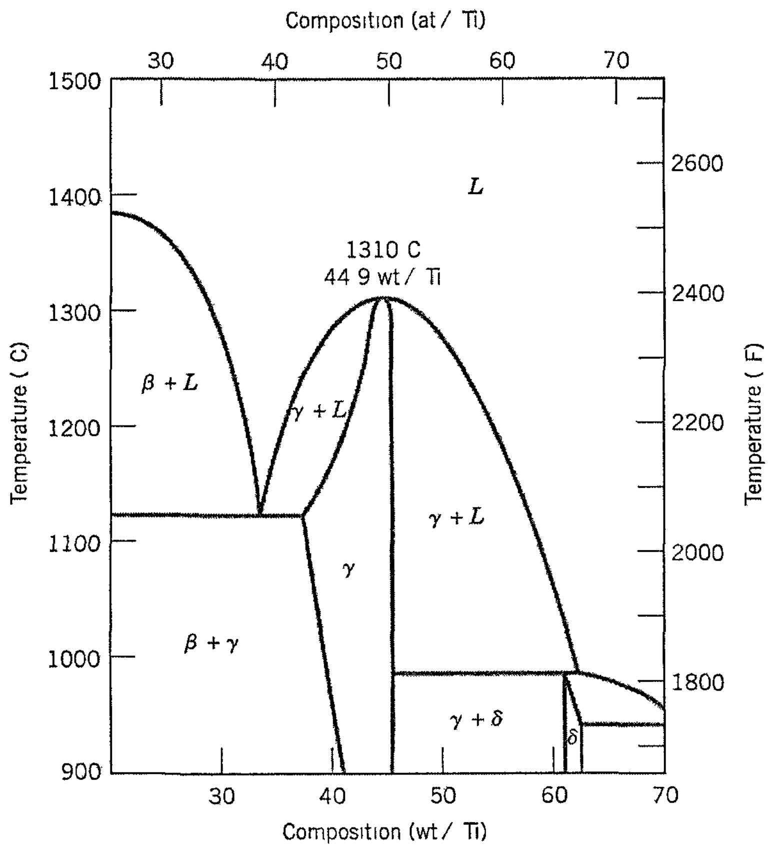
1 Polyethylene (PE) is generally a semi crystalline polymer meaning that it can be considered as a two phase structure consisting of A) amorphous and B) crystalline regions Calculate the theoretical densities of totally crystalline and totally amorphous polyethylene if the density of a 46% crystalline PE is 0 925 g/cm^3 and the density of an 80% crystalline PE is 0 972 g/cm^3 **(10 marks)**

2 Briefly explain why it is generally more difficult for a higher molecular weight polymer to crystallize **(2 marks)**

3 Estimate the average extended chain length for a sample of polypropylene if the average molecular mass is 35 000 g/mol The molar mass of C is A_C = 12 01 g/mol and the molar mass of hydrogen is A_H = 1 01 g/mol Assume a C C bond length of 0 153 nm and a C C bond angle of 109 5° **(8 marks)**

Question VII Phase Diagrams

A region of the Ni Ti equilibrium phase diagram is shown below For this question assume fully established phase equilibria at any given composition temperature combination as established during slow cooling



1 Identify all of the invariant reactions shown on this portion of the Ni Ti phase diagram their type and the temperature at which they occur **(6 marks)**

2 Describe the solidification sequence for a Ni 60wt %Ti alloy from a temperature of 1300 C **(4 marks)**

3 Sketch the expected microstructure for a Ni 60wt %Ti alloy at a temperature of 900°C if it was cooled from the liquid state and calculate the weight fraction of the phases present **(4 marks)**

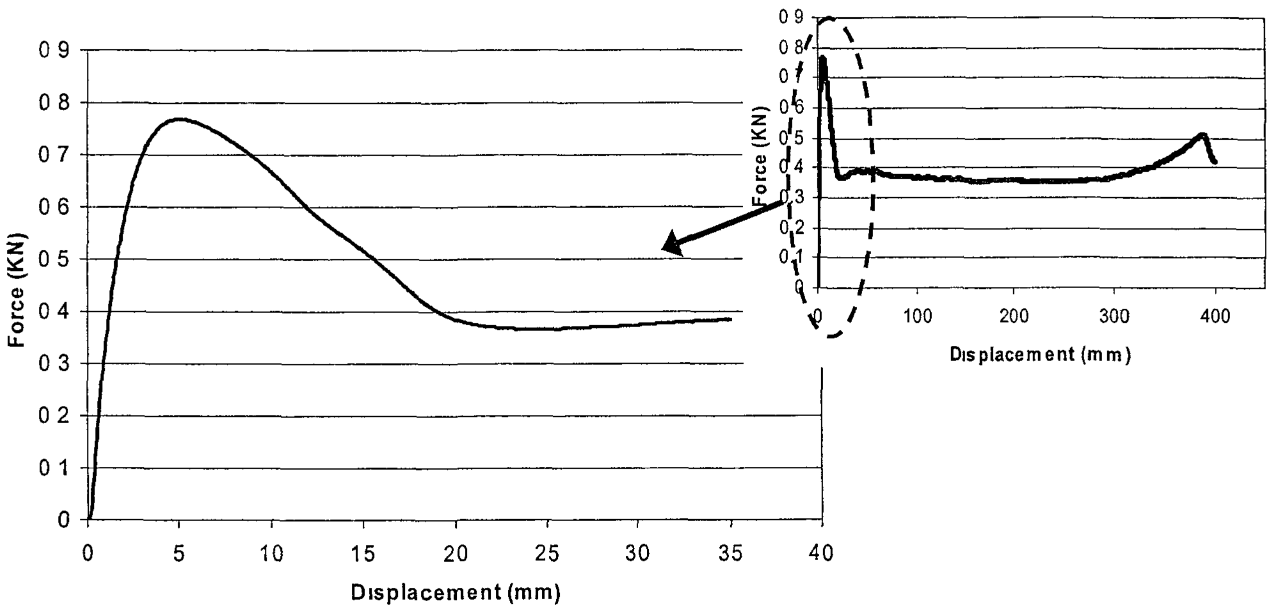
4 Sketch schematic diagrams of the potential energy as a function of interatomic spacing for the three solid phases shown on the phase diagram and briefly explain the expected differences between the curves **(4 marks)**

5 When heating slowly from room temperature at what temperature would the first liquid form for a Ni 68wt %Ti alloy? **(2 marks)**

Question VIII Mechanical Deformation

1 A single crystal of a metal that has the FCC crystal structure is oriented such that a tensile stress is applied parallel to the [1 0 0] direction If the critical resolved shear stress for this material is 0 5 MPa calculate the magnitude of applied stress necessary to cause slip to occur on the (111) plane in the [1 0 1] direction **(5 marks)**

2 Answer the following questions about the force displacement curves obtained from uniaxial tensile testing of a high density polyethylene sample having a gage cross section of 5 00 mm x 3 00 mm and gauge length of 60 mm **(3 marks each, 15 marks total)**



A) What is the elastic modulus of this material?

B) What is the yield strength (in units of MPa) of this material?

C) The width of the gage section was 5 00 mm before loading What would the width be under a load of 600 N? (Poisson s Ratio is 0 39)

D) Sketch the shape of the sample at displacements of 5 mm 50 mm and 350 mm

E) Why does the load increase again at displacements greater than 350 mm?

Appendix Equations and Constants

$$N_D = N\exp\left(-\frac{Q_D}{kT}\right) \qquad N = \frac{N_A \rho}{A} \qquad \varepsilon = \frac{\Delta l}{l_0} \qquad \sigma = \frac{F}{A_0}$$

$$E = 2G(1+\nu) \qquad \tau = G\gamma \qquad \sigma = E\varepsilon \qquad \tau = \frac{F}{A_0} \qquad \nu = -\frac{\varepsilon}{\varepsilon} = -\frac{\varepsilon_y}{\varepsilon}$$

$$U_r = \frac{\sigma_y \varepsilon_y}{2} = \frac{\sigma_y^{\,2}}{2E} \qquad \%EL = \left(\frac{l_f - l_0}{l_0}\right)\times 100 \qquad \%RA = \left(\frac{A_0 - A_f}{A_0}\right)\times 100 \qquad \sigma_T = \frac{F}{A_i}$$

$$\sigma_T = \sigma(1+\varepsilon) \qquad \varepsilon_T = \ln\frac{l}{l_0} \qquad \varepsilon_T = \ln(1+\varepsilon) \qquad \sigma_T = K\varepsilon_T$$

$$n\lambda = 2d\sin\theta \qquad d = \frac{a}{\sqrt{h^2+k^2+l^2}} \qquad \tau_R = \sigma\cos\phi\cos\lambda \qquad \sigma_y = \frac{\tau_{CRSS}}{(\cos\phi\cos\lambda)_m}$$

$$a = 2R \qquad a = 2\sqrt{2}R \qquad a = \frac{4R}{\sqrt{3}} \qquad APF = \frac{V}{V}$$

$$\rho = \frac{n\ (\Sigma A_C + \Sigma A_A)}{V_C\ N_A} \qquad \rho = \frac{n\ \ A}{V_C\ N_A} \qquad \theta = \cos^{-1}\left[\frac{u_1u_2 + v_1v_2 + w_1w_2}{\sqrt{\left(u_1^{\,2}+v_1^{\,2}+w_1^{\,2}\right)\left(u_2^{\,2}+v_2^{\,2}+w_2^{\,2}\right)}}\right]$$

$k = 1\ 38 \times 10^{23}\ \mathrm{J}/_{\mathrm{atom\,K}} = 8\ 62 \times 10^{5}\ \mathrm{eV}/_{\mathrm{atom\,K}}$ $\qquad$ $R = 8\ 31 J/mol\ \ K$

$T_K = T_C + 273$ $\qquad$ $e = 1\ 602\times10^{-19} C$ $\qquad$ $N_A = 6\ 023\times10^{23} mol^{-1}$