

National Exams May 2009

98-Met-A4, Structure of Materials

3 Hours Duration

NOTES

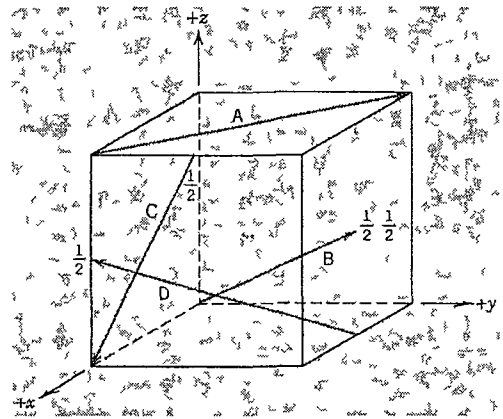
- 1 If doubt exists as to the interpretation of any question, the candidate is urged to submit with the answer paper, a clear statement of any assumptions made
- 2 Candidates may use one of two calculators, the Casio or Sharp approved models. This is a Closed Book exam. All equations, constants and diagrams 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

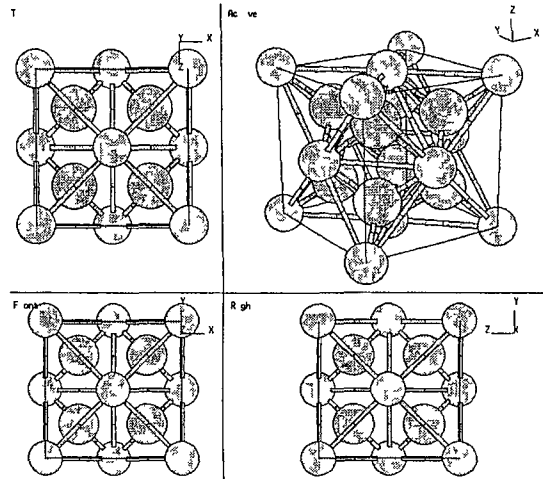
- The electron configuration of atomic Li ($Z=3$) can be expressed as $1s^2 2s^1$. Give the electron configurations for atomic Mg ($Z=12$) and Ti ($Z=22$) (4 marks)
- For the general case of an arbitrary atom, how many electron states are available in (i) the second shell, and (ii) the third shell? (i.e. how many electron states are possible when the principal quantum number n has values of $n = 2$ and $n = 3$)? (2 marks)
- The net potential energy E_N between two adjacent ions can be expressed by the equation $E_N = \frac{A}{r^{12}} - \frac{B}{r^6}$, where r is the interatomic separation and A, B are constants. Derive an expression for the equilibrium interatomic separation and the bonding energy (14 marks)

Question II Cubic Crystal Structures

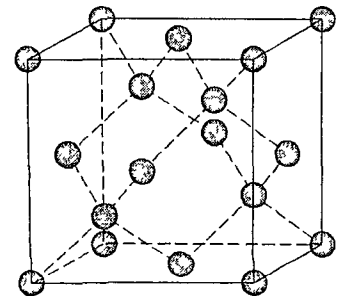
- Determine the indices for the four directions shown in the cubic unit cell shown right (4 marks)



- The calcium fluoride (CaF_2) crystal structure can be considered as a FCC lattice of Ca^{2+} cations with F^- anions located in the tetrahedral interstitial sites. Show by calculation that the CaF_2 unit cell is electroneutral (10 marks)

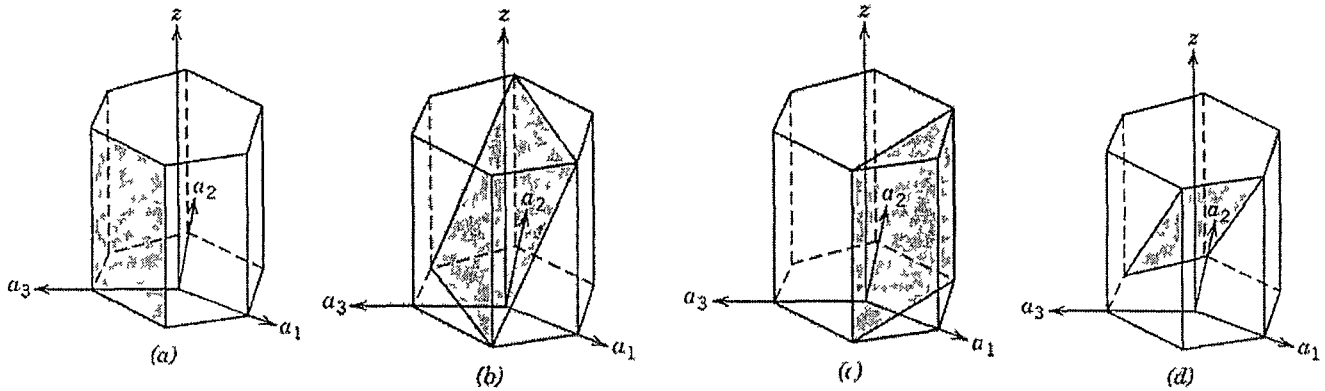


- The diamond structure is shown right. Its lattice constant is 0.357 nm. Calculate the theoretical density of diamond (For C $A_w = 12.01$ g/mol) (6 marks)

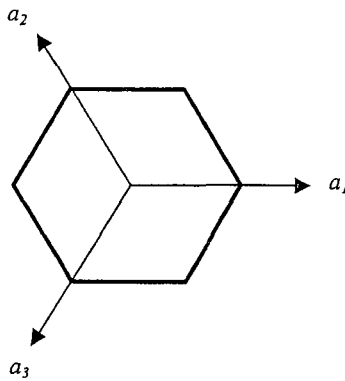


Question III Hexagonal Crystal Structures

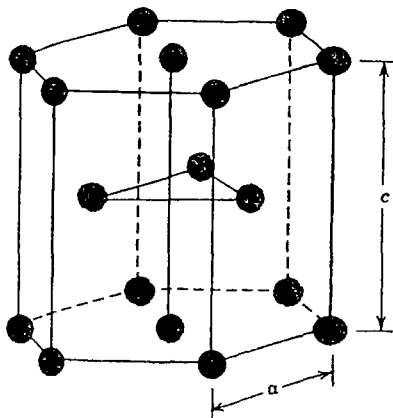
1 Identify the planes below in three and four index notation (4 marks)



2 Using a schematic diagram like the one shown below for the (0001) plane of a HCP unit cell, sketch the six directions that make up the $\langle 11\bar{2}0 \rangle$ family of directions, clearly labelling each direction (6 marks)



3 Show that the ideal c/a ratio for hexagonal close-packed structure is equal to $\sqrt{\frac{8}{3}}$ (10 marks)

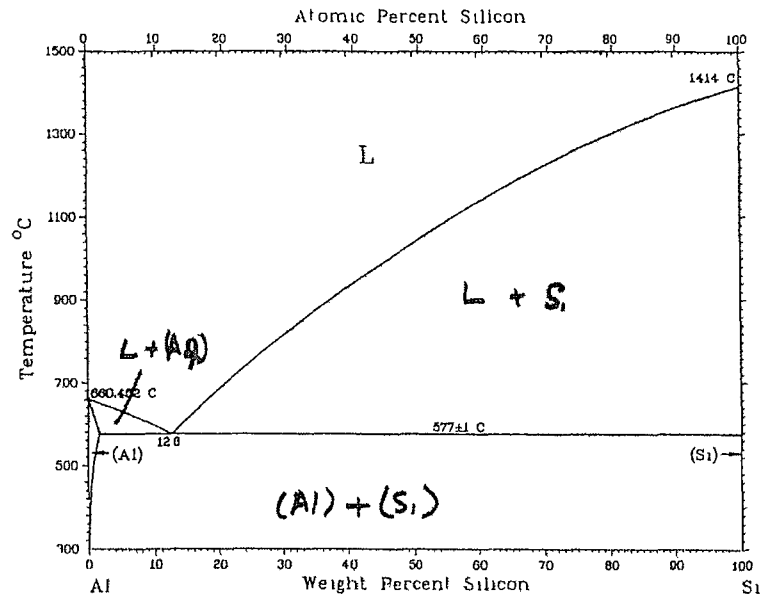


HCP

Question IV Phase Diagrams and Crystal Structures

Silicon and aluminum have very limited mutual solubility, which can be seen in the aluminum-silicon phase diagram shown right

1 Sketch a schematic diagram of the expected microstructure for a Al-50wt %Si alloy that has been slowly cooled from 1300 °C to just below the eutectic temperature. Give the composition of each phase, the weight fraction of each phase, and the weight fraction of the eutectic microstructure (5 marks)



2 Briefly explain why upon solidification an alloy of eutectic composition forms a microstructure consisting of alternating layers of the two solid phases (2 marks)

3 Determine the size of the octahedral and tetrahedral interstitial sites in aluminum (Al is FCC and has an atomic radius of 0.1431 nm). Hint: determine the size of the largest hard sphere that can fit undisturbed in the FCC lattice on the octahedral and tetrahedral sites (7 marks)

4 Determine the size of the tetrahedral interstitial sites in silicon (Si has the diamond cubic structure with a lattice parameter of 0.357 nm) (5 marks)

Question V X-ray Diffraction

Lead zirconate titanate ($\text{PbZr}_x\text{Ti}_{1-x}\text{O}_3$) is a piezoelectric crystal that will change shape under the influence of an applied voltage. When x is less than 0.5, lead zirconate titanate has a tetragonal primitive lattice with lattice parameters $a = 0.404$ nm and $c = 0.414$ nm. The interplanar spacing d for a tetragonal crystal structure can be expressed as

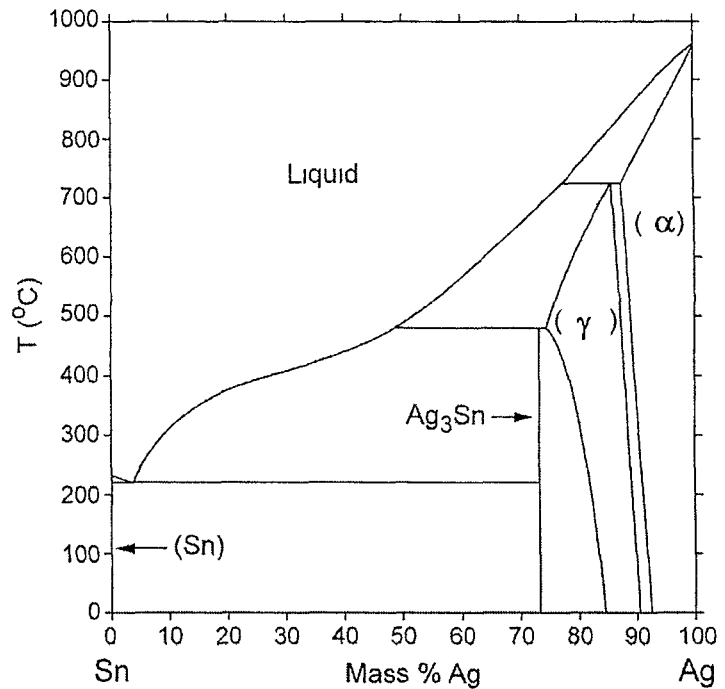
$$\frac{1}{d^2} = \frac{1}{a^2} (h^2 + k^2) + \frac{1}{c^2} l^2$$

Sketch a

schematic diagram of the expected powder diffraction pattern for $\text{PbZr}_{0.5}\text{Ti}_{0.5}\text{O}_3$ giving numerical values for the 2θ diffraction angle of the first five diffraction peaks (i.e. those planes corresponding to the five smallest 2θ values) if the $\text{PbZr}_{0.5}\text{Ti}_{0.5}\text{O}_3$ was characterized using $\text{Cu K}\alpha$ radiation ($\lambda = 0.154$ nm) (20 marks)

Question VI Phase Diagrams

Answer the following questions for the Sn-Ag phase diagram shown right



- 1 Clearly label any six of the seven two-phase regions on the phase diagram (6 marks)
- 2 Determine the concentration of each phase and the amount of each phase for a 30%Sn-70%Ag alloy at 600°C (4 marks)
- 3 Identify the invariant points (e.g. eutectoid) that are present in the Sn-Ag phase diagram and give the specific reactions involved (6 marks)
- 4 Identify the solidification sequence for a 20%Sn-80%Ag alloy that is cooled from the fully liquid state to ambient (4 marks)

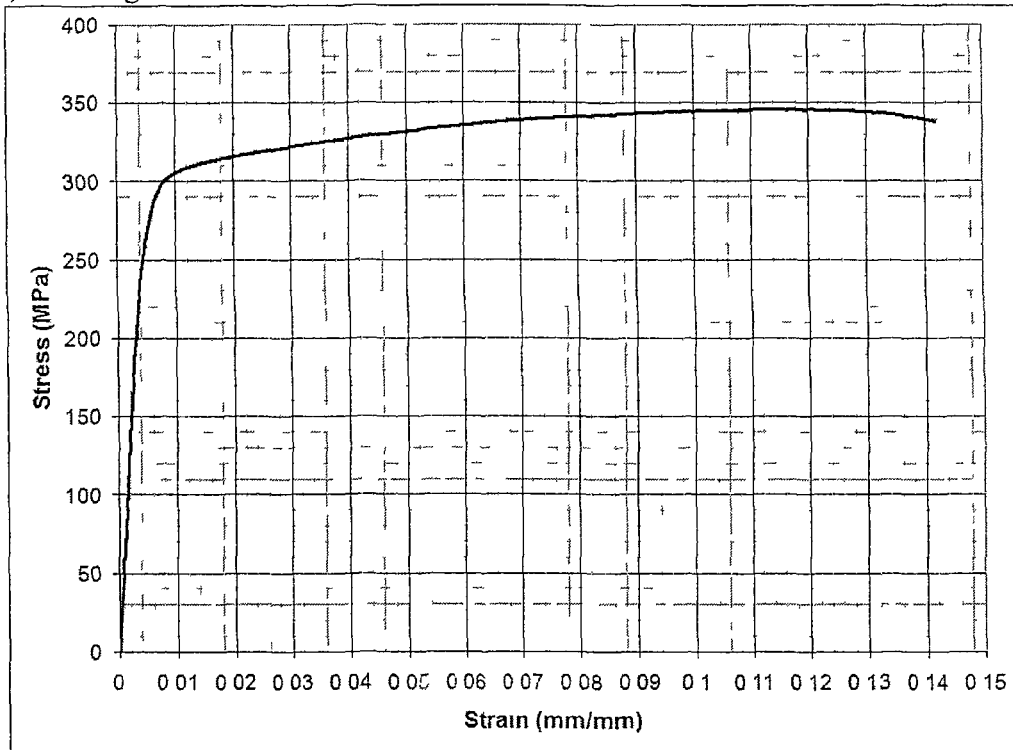
Question VII Point Defects

The Cu-Ni system is isomorphous, meaning there is complete solubility in the solid state over all temperatures and alloy compositions

- 1 Is the Cu-Ni solid solution substitutional or interstitial? Briefly explain your answer (3 marks)
- 2 There are several features of the solute and solvent atoms that determine the degree to which the solute can dissolve in the solvent. Briefly explain three of these factors (6 marks)
- 3 The equilibrium concentration of point defects often follows an Arrhenius-type temperature dependency. Calculate the fraction of (1) vacant lattice sites and (2) self-interstitial sites for nickel at its melting temperature of 1455°C. Assume an energy of 0.7 eV/atom for vacancy formation and an energy of 1.4 eV/atom for self-interstitial formation (4 marks)
- 4 Suppose that MgO was added as an impurity to Al₂O₃. If the Mg²⁺ substitutes for Al³⁺, (i) what kind of vacancies would you expect to form, and (ii) how many of these vacancies are created for every Mg²⁺ added? (4 marks)
- 5 Briefly explain the difference between a Frenkel and a Schottky defect (3 marks)

Question VIII Mechanical Deformation

A cylindrical bar of aluminum (100 mm original length and 15 mm original diameter) is loaded in tension, resulting in the stress-strain curve shown below



- 1 Using the stress-strain curve, give numerical values for the following properties: Young's modulus, proportional limit, 0.2% offset yield strength, tensile strength, ductility, and resilience **(6 marks)**
- 2 At what strain does the cross-section of the tensile coupon begin to decrease by i) uniform plastic deformation and ii) non-uniform plastic deformation? **(2 marks)**
- 3 What is the total elastic strain energy (in J) stored in the aluminum bar if a tensile load of 200 MPa has been applied? **(5 marks)**
- 4 Give the change in length and diameter (in mm) at a tensile load of 200 MPa. Assume a Poisson's ratio of 0.33 for aluminum **(4 marks)**
- 5 A) When an elastic tensile load is applied, the volume of a material having a Poisson's ratio of 0.33 will i) increase, ii) decrease, or iii) remain the same **(1 mark)**
B) When an elastic tensile load is applied, the volume of a material having a Poisson's ratio of 0.5 will i) increase, ii) decrease, or iii) remain the same **(1 mark)**
C) During elastic tensile deformation, the cross-sectional area of a material having a Poisson's ratio of less than zero will i) increase, or ii) decrease **(1 mark)**

Question IX Polymer Structures

For a linear polymer molecule, the extended chain length (L_{ext}) depends on the bond length between chain atoms (l), the total number of bonds in the molecule (m), and the angle between adjacent backbone chain atoms (109.5°), as follows

$$L_{ext} = ml \sin\left(\frac{109.5^\circ}{2}\right)$$

By contrast, the root-mean-square length, \bar{L} , is given by $\bar{L} = l\sqrt{m}$

- 1 A linear polystyrene $[-\text{CH}(\text{C}_6\text{H}_5)\text{CH}_2-]_n$ has an average molecular weight, \bar{M} , of 300,000 g/mole, compute average values of L_{ext} and \bar{L} for this material. The C-C single bond length is 0.154 nm and the C=C double bond length is 0.134 nm. **(10 marks)**
- 2 Briefly explain the reason for the difference in L_{ext} and \bar{L} . **(2 marks)**
- 3 For a linear polytetrafluoroethylene, $[-\text{CF}_2\text{CF}_2-]_n$ determine
 - A) The average molecular weight for $L_{ext} = 2000$ nm, **(4 marks)**
 - B) The average molecular weight for $\bar{L} = 15$ nm **(4 marks)**

Appendix Equations and Constants

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

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

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

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

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

$$a = 2R \quad a = 2\sqrt{2}R \quad a = \frac{4R}{\sqrt{3}} \quad APF = \frac{V_s}{V_c}$$

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

$$k = 1.38 \times 10^{-23} \text{ J/atom K} = 8.62 \times 10^{-5} \text{ eV/atom K} \quad R = 8.31 \text{ J/mol K}$$

$$T_K = T_C + 273 \quad e = 1.602 \times 10^{-19} \text{ C} \quad N_A = 6.023 \times 10^{23} \text{ mol}^{-1}$$