NATURAL SCIENCES TRIPOS Part IA

Friday 8th June 2001 1.30 to 4.30

MATERIALS AND MINERAL SCIENCES

Answer ***five*** *questions;* ***two*** *from each of sections A and B and* ***one*** *from section C.*

Begin each answer at the top of a sheet.

Write on ***one*** *side of the paper only.*

Graph paper and the Data Book are provided.

Candidates using electronic calculators are advised to indicate clearly the sequence of steps in their working. Appropriate credit can then be given for the intermediate stages, even if the final stage is incorrect.

The answer to ***each question*** *must be tied up* ***separately****, with its own cover-sheet.*

Write the relevant ***question number*** *in the square labelled 'Section'. Also, on* ***each*** *cover sheet, list the numbers of* ***all*** *questions attempted.*

You may not start to read the questions printed on the subsequent pages of this question paper until instructed that you may do so by the Invigilator

SECTION A

1 Explain the meaning of the terms: *slip system, yield stress,* and *resolved shear stress*.

Sketch a typical tensile stress vs strain curve for the deformation of a single crystal ccp metal. Mark on your diagram the region of elastic deformation, and the three stages of plastic deformation. Explain the microstructural processes occurring during each stage. Compare your diagram with that which would be obtained for a polycrystalline metal. How is the critical resolved shear stress (τ_c) related to the tensile yield stress (σ_y) in a polycrystalline material?

What is Schmid's law? - define the terms involved and hence calculate the resolved shear stress acting upon $[1\bar{1}0]$ (111) for a 5 kPa tensile stress applied parallel to $[2\bar{1}4]$. Determine the slip system with the greatest Schmid factor, and calculate the resolved shear stress acting on this system.

During slip, dislocations may interact. Consider the interaction between $\mathbf{b}_1 = \frac{a}{2}[\bar{1}10]$ moving on (111) and $\mathbf{b}_2 = \frac{a}{2}[10\bar{1}]$ moving on $(1\bar{1}1)$. Using Frank's rule, show that it is energetically favourable for these dislocations to add. Describe the character of the resultant dislocation. What is the significance of the new slip system in terms of continued plastic deformation?

2 Explain what is meant by a brittle solid. Why do most ceramics behave in a brittle manner?

Derive the Griffith criterion for a fixed plate containing an internal through thickness crack of length 2a. The thickness of the plate is t, and it is subject to a remote stress, σ, perpendicular to the crack face. Explain carefully any assumptions you make, and the effect these assumptions will have on the result.

A large pressure vessel in a chemical plant operates at an internal pressure P_{max} = 3 MPa. The vessel has a diameter of 4 m and is made of steel with a thickness of 8 mm. The steel has a yield strength of 800 MPa and a fracture toughness, K_c = 70 MPa $\sqrt{m}$. The pressure vessel is regularly inspected to check for cracks in the steel. The inspection procedure can reliably detect any cracks above 0.5 mm in length. Is it safe to operate the pressure vessel under these conditions?

3 Define the term *lattice*, and explain the difference between the use of *primitive* and *non-primitive* unit cells.

Tungsten can be prepared in a cubic structure, a = 5.1 Å, with atoms in two types of position:

W(1): 000; $^1/_2,^1/_2,^1/_2$

W(2): $0,^1/_2,^1/_4$; $^1/_4,0,^1/_2$; $^1/_2,^1/_4,0$; $0,^1/_2,^3/_4$; $^3/_4,0,^1/_2$; $^1/_2,^3/_4,0$

Draw a plan of 2 x 2 unit cells viewed down [001]

(i) Determine the lattice type.

(ii) Does the structure have a centre of symmetry?

(iii) List the directions and positions of any rotation axes.

(iv) List the orientations and positions of any mirror planes.

(v) Describe the coordination of one of the W(1) atoms and calculate the distance to its neighbour atoms.

4. Define the term *coordination polyhedron* and explain why it is a useful concept in understanding the structure and properties of ionic materials. Illustrate your answer with reference to the cubic NaCl, CsCl and ZnS structures.

Calculate the minimum radius ratios $\left(\frac{r^+}{r^-}\right)$ for each of these structures.

Estimate, giving reasons, an upper limit for the stability of the CsCl structure in alkali metal/halide systems. The ionic radius of Cs^+ is 1.81 Å and the radii of the halide anions are: F^- = 1.19Å, Cl^- = 1.67 Å, Br^- = 1.82 Å and I^- = 2.00 Å. Which Cs halides will be stable within the CsCl structure?

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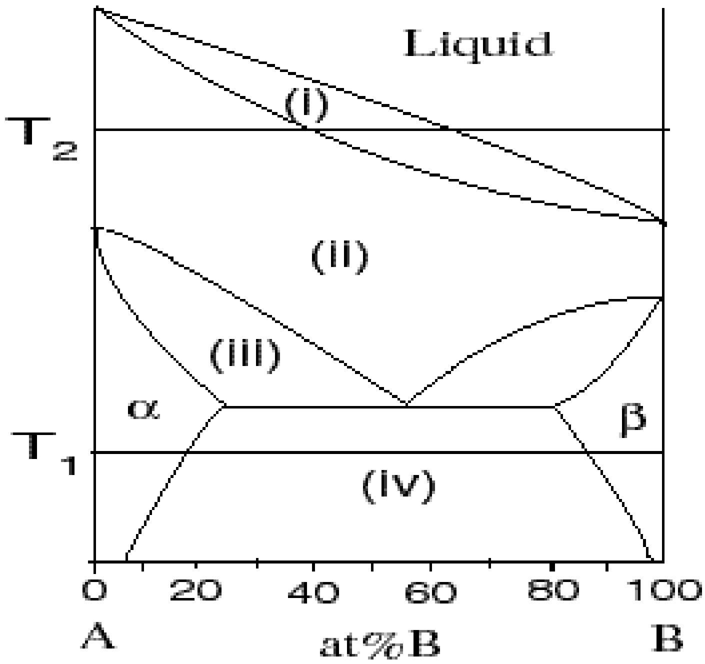
SECTION B

5 What is meant by the terms *solid solution* and *phase separation*? Draw simple phase diagrams to illustrate your answer. Include sketches of free energy curves at various temperatures to explain the features of the phase diagrams.

The diagram below shows the phase behaviour of elements A and B as a function of temperature. Describe the phases present in each of the regions marked (i) – (iv). For compositions of 5 at %B and 55 at %B describe the composition of the phases present and the relative amounts at temperatures T_1 and T_2.



For compositions of 5 at %B, 30 at %B and 55 at %B sketch and describe the microstructures you would expect for slow cooling from high temperature down to temperature, T_1. Indicate how rapid cooling would change the microstructure in each case.

6 Explain what is meant by a material being *anisotropic* with respect to a particular property. Describe *Neumann's principle* and how we can use it to predict the anisotropic behaviour of materials.

The mineral zircon is tetragonal and has refractive indices n_o = 1.923 , n_e = 1.967. Sketch the representation surface that describes the propagation of light through a crystal of zircon, indicate the orientation of the optic axis. For light impinging normally onto the (013) face of a zircon crystal, give the polarisation directions [uvw] of the two light rays and the associated refractive indices. What thickness of zircon cut parallel to this crystal face would result in a first order yellow colour being observed between crossed polarisers in white light? Give a brief explanation of why yellow is the first *complementary* colour.

[zircon: a = 6.60Å, c = 5.98Å; from Michel-Levy chart, retardation equivalent to yellow = 350 nm]

7 Describe how the *powder diffraction method* is used to determine the structure of materials.

WO_3 has a cubic structure. The first few peaks in a powder diffraction measurement were recorded at the following scattering angles using Cu Kα radiation:

23.73° 33.80° 41.72° 48.55° 54.73° 60.50° 71.14°

Determine the lattice type and the lattice parameter.

WO_3 undergoes a displacive phase transition to a tetragonal structure. Assuming that the new *c*-lattice parameter is slightly larger than the new *a* lattice parameter, describe the changes in the diffraction pattern associated with the first 4 peaks if they are influenced by multiplicity only.

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8 A transmission electron microscope can be operated to show either an image or the diffraction pattern of the specimen. Draw a schematic diagram to include the specimen, the objective lens, the back focal plane and the image plane and show the principle behind the modes of operation.

Using this diagram show how the microscope would be operated to give *bright field* and *dark field* images.

Iron meteorites consist of a Ni-rich (fcc) and Fe-rich (bcc) phase formed upon cooling. A *dark field* image of a meteorite specimen is produced using a diffracted beam 21.6 mm from the optic axis and is shown to be the Ni-rich phase. A second *dark field* image using a spot 18.1 mm from the optic axis in the same direction as the first is found to produce an image of the Fe-rich phase. In the same diffraction pattern a similar relationship exists for diffraction spots at 35.34 mm (Ni-rich) and 44.30 mm (Fe-rich) from the optic axis. Identify the lattice planes giving rise to each of these reflections and suggest a reason for the orientation relationship observed.

[λL = 36.75 mm Å, $a_{Ni\text{-}rich}$ = 2.94Å, $a_{Fe\text{-}rich}$ = 2.87 Å]

SECTION C

9 Describe the different scales of structure which arise in *cortical bone*.

Tensile test specimens with a gauge length of 25.4 mm, a width of 18.0 mm and a thickness 2.0 mm, were prepared from tibial cortical bone, with the tensile axis oriented parallel to the long axis of the bone. The specimens were deformed to fracture, at a constant strain rate of 3×10^{-4} s^{-1}, at 37 ˚C in a physiological environment. For 5 specimens, the test results were: Young's Modulus (E) = 25 ± 1 GPa, Ultimate Tensile Strength (UTS) = 110 ± 40 MPa. Comment on the testing methodology, sketch the stress-strain curve and discuss the significance of the values of E and UTS.

The same testing procedure was repeated, but with a sharp notch machined on one edge of the tensile specimen to introduce cracks of length (a): 1.25, 3.00 and 6.00 mm. The associated values of fracture stress (σ_{Fr}) were 60.0, 33.0 and 21.0 MPa. Discuss how the relationship between (σ_{Fr}) and (a) can be modelled. Use this relationship to derive the critical crack lengths associated with fracture in the un-notched tensile specimens and relate this to microstructural features. How could a microstructural feature of equivalent dimension act as a *crack stopper*?

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10 Answer **two** of the following (a), (b) or (c):

(a) Compare the two ways in which precipitate particles in an alloy may inhibit dislocation motion?

On annealing a particular magnesium alloy, ultra-hard precipitate particles develop in its Mg-based matrix. After a long anneal, the volume fraction of the precipitate phase in the alloy is 6%, and the individual particles have a spherical radius of 10 nm. Make a quantitative estimate of the critical resolved shear stress for slip in this annealed alloy.

[For magnesium, G = 17.3 GPa]

(b) Briefly outline the experimental methods that may be used to determine the pressure temperature phase diagram of a particular material.

The transformation from one polymorph to another of Al_2SiO_5 is studied as a function of temperature and pressure. On heating the polymorph Andalusite at a constant pressure of 0 MPa, it transforms to Sillimanite at 1048 K; this transformation is endothermic with a latent heat of 3122 J mol^{-1}. On pressurising Andalusite at a constant temperature of 300 K, it transforms to Sillimanite at 1466 MPa.

Evaluate the entropy difference between the two polymorphs. Andalusite has a molar volume of 5.158×10^{-5} m^3 mol^{-1}; what is the molar volume of Sillimanite?

(c) The flat panels of an aircraft skin would preferably be of a material chosen to give minimum weight for a given elastic deflection; the merit index for this case is $E^{1/3}/\rho$. Describe how this index can be used with the appropriate materials selection map to rate materials. Of different engineering alloys, those based on which element would be best for this application? Alloys of which element are commonly used? Comment on the possible reasons for this choice.

A wire is suspended from one end. Which is the merit index for selection of the material which would give the longest wire supporting its own weight without yielding? Of common polymeric, metallic and ceramic materials which would be best and worst for maximising this limiting length.

END OF PAPER