NATURAL SCIENCES TRIPOS Part IA

Friday 4 June 1999 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.*

SECTION A

1 Explain the meanings of the terms *crystal system* and *Bravais lattice.*

Above 250˚C, the mineral perovskite, $CaTiO_3$, has the cubic perovskite structure with lattice parameter a = 3.88 Å. Below this temperature, the structure distorts slightly to an orthorhombic form with lattice parameters a = 5.48 Å, b = 3.87 Å and c = 5.47 Å.

(a) Draw a projection of four unit cells of the cubic perovskite structure on (001), sharing a common edge. Describe the coordination of Ti and Ca atoms by oxygen, and describe the structure in terms of the arrangement of Ti coordination polyhedra.

(b) Draw a sketch plan to illustrate the relationship between the cubic and orthorhombic forms of $CaTiO_3$, labelling the axes.

(c) A single grain of the cubic phase transforms to the orthorhombic phase. How many possible twin orientations could develop?

(d) The indices of lattice planes change on the transformation from the high- to the low-temperature structure. What would the indices of the cubic (101), (200) and ($\bar{1}$10) planes become in the orthorhombic structure?

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2 Describe the atomic scale structural differences between crystals and glasses. State three physical properties which would differ significantly between these two states and explain the differences in structural terms.

Draw a sketch plan of the atomic structure of crystalline silicon (diamond structure, a = 5.42 Å). Determine the multiplicity of the <110>, <111> and <311> lattice vectors in silicon. Establish the number and distances of neighbours in each of these three sets of directions and hence sketch the radial distribution function, $g(r)$, for crystalline Si for r < 4.5 Å. Sketch the corresponding $g(r)$ plot for amorphous silicon.

3 Define the terms *neutral axis*, *bending moment* and *flexural rigidity* for a loaded elastic beam.

Sketch a solid square-sectioned beam supported on knife edges a distance L apart and loaded vertically mid-way between the supports. Mark on your sketch the locations in the beam where (a) the tensile stress is greatest, (b) the compressive stress is greatest, and (c) there is no stress.

The vertical displacement δ of the centre of the beam under a load W is given by

$$\delta = \frac{W L^3}{48 E I}$$

where E is Young's modulus and I is the second moment of area of the cross-section. For a certain application, a solid square-sectioned beam with a fixed length and density ρ must have a fixed stiffness (W/δ). Derive a function of E and ρ which must be maximised for the beam to have minimum mass. What other properties might be important is selecting a material for a beam to form part of a road bridge? How might the design of the beam be modified to reduce its mass further while retaining its stiffness?

4 Show that a simple model for the critical shear stress τ_c needed to cause slip in a perfect crystalline material predicts

$$\tau_c = \frac{G\beta}{2\pi h}$$

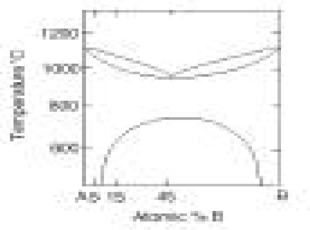
where G is the shear modulus, β is the interatomic spacing in the shear plane and h is the interplanar spacing. Hence estimate the value of τ_c in terms of G for a cubic close-packed material. Why do most crystalline materials yield at shear stresses which are several orders of magnitude lower than the value predicted by this model?

The axis of a cylindrical single crystal of silver, of cross-sectional area 5 mm^2 and initial length 50 mm, lies in the planes $(30\bar{1})$ and $(11\bar{1})$. The sample yields at a tensile load, applied along its axis, of 20 N. Calculate the critical resolved shear stress for this material.

The crystal is deformed until a second slip system comes into operation. Determine the crystallographic orientation of the tensile axis and the length of the specimen at this point.

SECTION B

5 Copy the following phase diagram and mark on it the *liquidus*, *solidus* and *solvus* lines and all the phase fields.



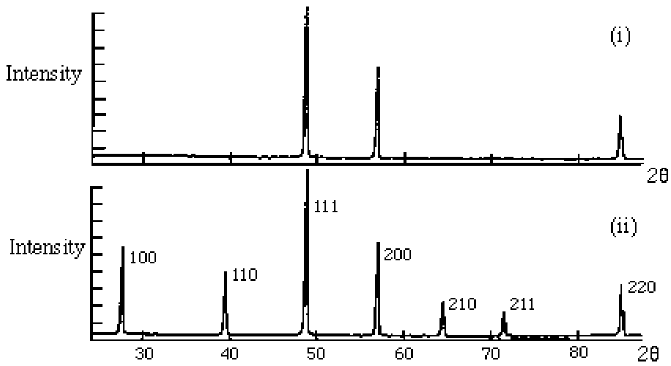
(a) Draw and label schematic free energy versus composition curves corresponding to temperatures of 1200˚C, 1000˚C, 800˚C and 600˚C.

(b) Sketch cooling curves for materials of compositions 5, 15 and 45 at%B during slow cooling from 1200˚C to 400˚C. Give the compositions and relative amounts of each phase for 45at%B at a temperature of 600˚C.

(c) How would the phase diagram change if the free energy of the liquid phase were substantially lower?

6 What is meant by a *reciprocal lattice*? Explain how the *Ewald sphere* construction can be used to predict the conditions under which diffraction will occur. Outline how *systematic absences* arise in a diffraction pattern. Sketch the section containing *b** and *c** of the reciprocal lattice, for cubic crystals having (a) a P lattice, (b) an I lattice and (c) an F lattice.

The powder diffractometer traces shown in the figure were obtained from an alloy of Cu_3Au (cubic), with the sample held at (i) 500˚C (top) and (ii) 300˚C (bottom). What is the lattice type of the alloy at each temperature? Account for the difference in terms of the distribution of atoms in the two cases. Why are there substantial variations in the heights of different peaks in the traces?



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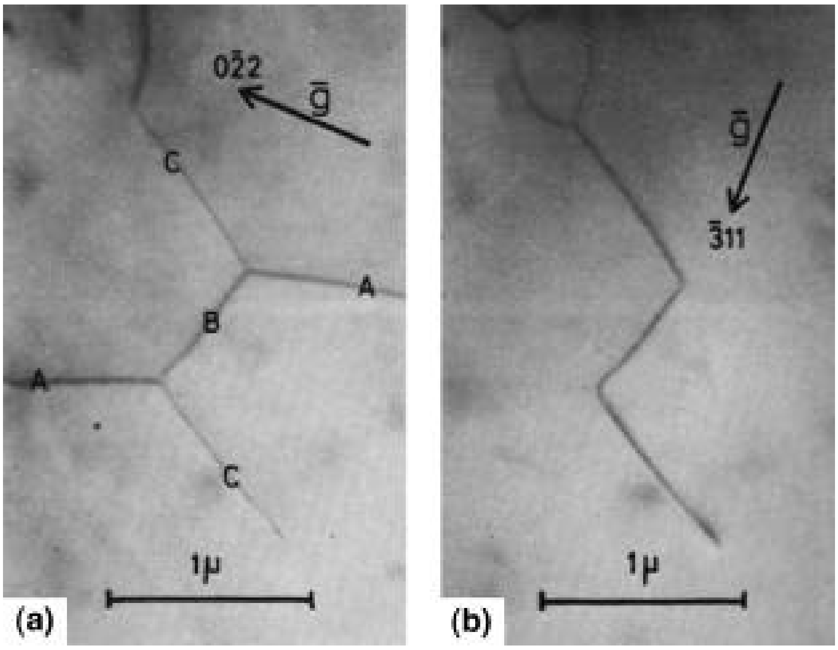
7 Explain briefly how (a) a diffraction pattern and (b) an image are formed in the transmission electron microscope. Distinguish between a *bright field image* and a *dark field image*. Outline how the presence of dislocations in a crystal leads to contrast in a TEM image.

The two micrographs shown below were obtained from a thin foil of Si (cubic F), with the same region being imaged in each case, but with the specimen tilted at different angles to the electron beam. The reciprocal lattice vector, **g**, indicated in each micrograph specifies the normal of the lattice planes which are diffracting most strongly. A network of three perfect dislocations is present in the region, all lying in the same plane. It is known that the dislocation marked as C in micrograph (a) has a Burgers' vector of $\frac{a}{2}[\bar{1}\,10]$. Establish the Burgers' vector for the dislocation marked as B in micrograph (a), explaining your reasoning.



8 Describe the appearance of a quartz wedge viewed in the 45˚ position between crossed-polars in (i) monochromatic light and (ii) white light. In each case explain the reasons for the effects seen.

A wedge of quartz cut with length *fast* and wedge angle 0.4˚ is viewed in sodium light (λ = 589 nm) between crossed-polars in the 45˚ position. Determine the distance between the dark bands. When a stretched polymer tape of thickness 150 µm is laid on top of the quartz wedge (with the stretch direction along its length), the bands are seen to move by 0.3 mm. When observed in white light between crossed-polars, only a single black band is observed. Determine the birefringence of the tape and its optic sign. Comment on the likely structure of the polymer, given your results.

SECTION C

9 Outline briefly what is meant by *entropy* and discuss its role in the thermodynamics of phase transformations.

Explain why the application of pressure to a system may lead to a change in the phase which is thermodynamically most stable. By considering the free energy change on melting a pure material at constant temperature and pressure, show that the entropy of fusion is given by the ratio of the latent heat of fusion to the equilibrium fusion temperature.

A large part of Antarctica is covered with a thick (~2 km) layer of ice. Concern is expressed that a relatively small rise in the temperature of the ice at the base of this layer, combined with the pressure being applied by the mass of ice above it, may cause melting, which could make parts of the ice pack unstable and likely to slide over the underlying rock into the sea. The temperature at the base of the ice pack is typically about -30˚C. Stating your assumptions, estimate the depression of freezing point arising from the applied pressure in this region and hence deduce whether the concern is justified.

[Latent heat of melting of ice = 340 MJ m^{-3}
Icebergs float with about $\frac{8}{9}$ of their volume below water level]

10 Answer both parts (a) and (b).

(a) Define the terms *diffusion creep* and *dislocation creep*. Sketch a diagram showing the dominant mechanisms of creep in a metal as a function of applied stress and temperature. What microstructural features are present in a nickel alloy for gas turbine blades to reduce creep deformation?

(b) Sketch the appropriate part of a binary phase diagram for an alloy which might exhibit age hardening and explain what features of the diagram are important. Precipitate particles nucleate in a particular Al-Cu alloy, under certain ageing conditions, at a constant rate of 2.5×10^{17} m^{-3} s^{-1}. Estimate the critical resolved shear stress of this alloy after ageing for 1 day. State your assumptions clearly.

[Shear modulus of aluminium = 26 GPa]