NATURAL SCIENCES TRIPOS Part IA

Friday 5 June 1998 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.

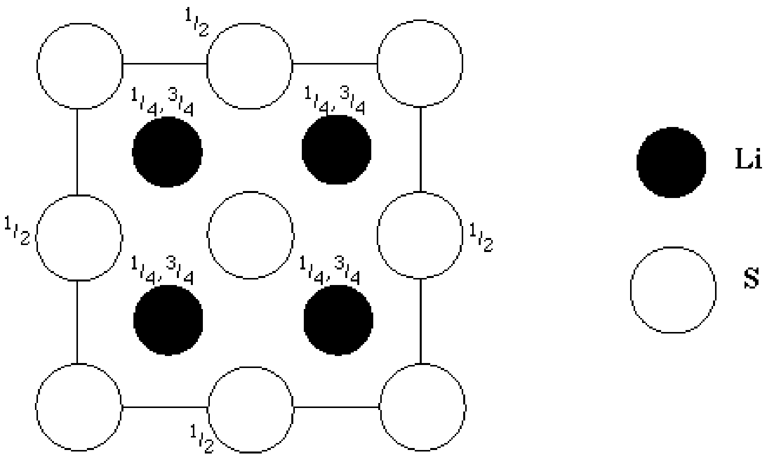
Candidates using electronic calculators are advised to indicate clearly the sequence of steps in their working. Appropriate credit can then be given for the intermediate stages, even if the final stage is incorrect.

*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 The figure below shows a plan view of the structure of lithium sulphide, Li_2S (cubic, a = 5.70 Å).



(a) What is the lattice type?

(b) How many formula units are there in this unit cell?

(c) What is the lattice motif?

Describe the coordination of S by Li and Li by S. Hence, comment on the packing of the S ions and the location of the Li ions. Compare this arrangement with that of NaCl.

Show that the smallest ion which could be accommodated in a site such as the Li site in Li_2S has a cation/anion radius ratio of 0.225. Comment on the validity of this approach to predicting the coordination of a cation.

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2 Explain carefully the meaning of the terms *rotation axis of symmetry, mirror plane* and *centre of symmetry*. Draw a plan on (001) of cubic $BaTiO_3$ (perovskite structure) showing a 2 × 2 block of unit cells with a common vertical edge. Add to one unit cell of the plan the traces of the mirror planes containing [001]. Identify the rotation axes parallel to [001] that pass through $\frac{1}{2}\,\frac{1}{2}\,0$ and $\frac{1}{2}\,0\,0$. Write down the coordinates of one of the centres of symmetry.

The properties *pyroelectricity*, *piezoelectricity* and *ferroelectricity* all involve the production of a dipole moment. Explain carefully the difference between these properties and discuss how a knowledge of the symmetry elements shown by a crystalline compound will indicate whether or not that compound may display one of these properties.

Above 120˚C, $BaTiO_3$ is cubic with a = 3.906 Å. At 120˚C, it undergoes a displacive transition to a tetragonal phase with a = 3.994 Å and c = 4.033 Å. In what direction is the Ti^{4+} ion displaced in the tetragonal form? Indicate how the symmetry elements of the tetragonal cell are related to those of the cubic cell.

Assuming that the ions are fully ionised, estimate the net polarisation per unit volume of the tetragonal phase, given that the displacements of the ions, relative to the O^{2-} ions with the same z coordinate as the Ti^{4+} ion in the cubic phase, are as follows: Ti^{4+}: +11 × 10^{-12} m; Ba^{2+}: +6 × 10^{-12} m; O^{2-}: –3 × 10^{-12} m.

3 Explain briefly what is meant by a *dislocation.* Outline the difference between an *edge* and a *screw* dislocation. What is meant by a *mixed* dislocation?

Derive the expression (*Schmid's law*) relating the tensile stress applied to a single crystal at the onset of yielding, σ_Y, to the critical resolved shear stress, τ_C, of the material and the angles between the tensile axis and the slip direction, λ, and between the tensile axis and the slip plane normal, φ.

A single crystal of high purity aluminium is produced in the form of a wire, with the [125] direction parallel to the wire axis. During tensile testing of the wire, plastic deformation is observed to start at an applied tensile stress of 8 MPa. Calculate the critical resolved shear stress.

Explain why the applied stress at the onset of yielding would differ if the aluminium were:

a) a single crystal of lower purity,

b) polycrystalline.

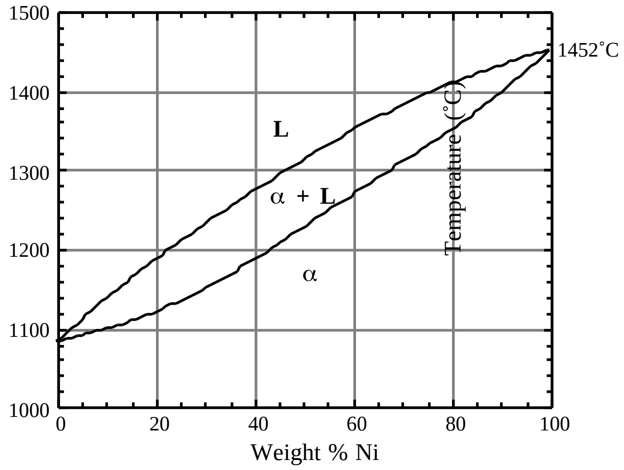
4 Define the *critical strain energy release rate* (or *toughness*) G_c of a material. To what extent is it possible to estimate the value of G_c for different materials from a knowledge of their surface energy γ ?

Define the term *Peierls stress*, τ_p, and explain how the variation of τ_p with temperature differs for a typical ccp metal and a typical bcc metal. Explain why a structural steel (e.g. Fe - 0.2 wt% C), as used for example in shipbuilding, exhibits a ductile-brittle transition at low temperatures. What features on a fracture surface might indicate the type of failure which had occurred?

A certain structural steel has a tensile yield stress of 200 MPa and a fracture toughness, K_c, of 40 MPa $m^{1/2}$, both at a temperature of 0˚C. Estimate the overall length of a crack, present through the thickness of the interior of a large plate, which would lead to brittle failure of this steel under a sufficiently high tensile load. Would such a steel be suitable for constructing a ship which might be involved in collision with an iceberg?

SECTION B

5 Briefly outline the meanings of the terms *phase*, *solid solution* and *coring* (or *zoning*). Derive the *lever rule*, which relates the equilibrium compositions of the phases present in a two-phase region of a phase diagram to the proportions of the two phases and the overall average composition of the alloy.



The above figure shows the phase diagram for the Cu-Ni system. Sketch approximate free energy - composition curves for the two phases present in this system, at temperatures of (a) 1000 ˚C, (b) 1200˚C and (c) 1452˚C. In each case, indicate the ranges of overall composition for which the phases are stable.

Estimate the percentage of solid phase present in an alloy of Cu-60 wt%Ni after prolonged heating at a temperature of 1300˚C.

An alloy of Cu-60 wt%Ni is being cooled from 1500˚C. Sketch the form of the cooling curve, down to 1000˚C. What effect would changes in the rate of heat extraction during cooling have on the final microstructure?

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6 Give a brief account of the powder method in X-ray diffraction. Explain how this method may be used to:

(a) calculate accurate values of the lattice parameters,

(b) determine the Bravais lattice of a cubic compound and

(c) follow the displacive phase transition from α-cristobalite (cubic) to β-cristobalite (tetragonal).

The θ angles in the table below were measured for the high - angle lines on a powder pattern of a cubic substance with $a \approx 3.6$ Å obtained with CoK_α radiation. Determine (i) the indices of the reflections, (ii) the lattice type and (iii) an accurate value of the lattice parameter.

$\theta\ (K_{\alpha_1})$	$\theta\ (K_{\alpha_2})$
44.54°	44.67°
55.31°	55.50°
59.17°	59.37°
82.32°	83.30°

7 Explain what is meant by the terms *reciprocal lattice* and *Ewald sphere*. Show how these concepts may be used to (a) interpret electron diffraction patterns from a thin crystal and (b) explain the formation of a dark field image of the crystal.

Spinel Mg_2AlO_4 has a cubic F lattice (a = 8.09 Å). Sketch the appearance of the electron diffraction pattern observed when the incident electron beam is parallel to [010], indexing the reflections with h, k and l all positive and $h^2 + k^2 + l^2 \leq 32$. Calculate the angle through which the crystal would have to be tilted in order to obtain an optimum dark field image, using the 404 reflection and electrons of wavelength 0.04 Å.

Two dislocation lines, AB and BC were observed in a series of dark field images as follows:

Most strongly diffracting reflection	Dislocation AB	Dislocation BC
400	invisible	visible
$00\bar{4}$	visible	invisible
404	visible	visible
$1\bar{1}3$	visible	invisible
$31\bar{1}$	invisible	visible

Determine the Burgers vectors of the dislocations AB and BC.

8 What is the difference between an *isotropic* and an *anisotropic* property of a material? Explain the use of the optical indicatrix in describing the optical properties of uniaxial crystals. Define the terms *birefringence* and *optically positive.*

A quartz wedge of angle 0.4˚ is placed in the 45˚ position between crossed-polarisers and viewed using monochromatic yellow light (λ = 589 nm). At what distances along the wedge are the first three positions at which dark fringes appear?

A strip of polycarbonate film, 0.1 mm thick and initially optically isotropic, is placed parallel to and partially overlapping the quartz wedge and the arrangement is now viewed in white light. The strip is stretched elastically along its length. The overlapping polycarbonate film and quartz wedge show a black band 1.9 mm along the wedge. What is the tensile stress applied to stretch the film? Is the length of the quartz wedge parallel or perpendicular to the *fast* direction?

SECTION C

9 Explain how substances displaying *displacive* and *reconstructive* phase transitions differ with respect to:

(a) the symmetry relationship between the phases,

(b) their response to quenching and

(c) the relative movement of atoms in the structure during the transformation.

Tin undergoes a reconstructive transformation from the β phase, white tin, to the α phase, grey tin, at low temperatures. The equilibrium temperature for the transition at atmospheric pressure is 13.2˚C. Use the data below to calculate

(i) the molar volume of each phase at 13.2˚C in units of $m^3\ mol^{-1}$ and

(ii) the pressure at which the transition temperature would be –20˚C.

It is found that white tin can be held for many years at a temperature of 0˚C at atmospheric pressure without significant transformation occurring to the grey allotrope. Suggest possible reasons for this.

[Grey tin (α phase) has the diamond structure, with a = 6.489 Å.
White tin (β phase) has a tetragonal-I lattice, with a = 5.832 Å, c = 3.181 Å and 2 atoms per lattice point. At 13.2˚C, S_α = 2.52 J K^{-1} mol^{-1} and S_β = 2.95 J K^{-1} mol^{-1}.]

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10 Explain the following observations as fully as possible.

(a) Increasing the grain size of a metal leads to a decrease in its yield stress. Gas turbine blades, however, are deliberately made with a very large grain size, or even as single crystals.

(b) The highest yield stress in a plain carbon steel (i.e. Fe - C) is achieved by quenching it from high temperature, but subsequent heating at a lower temperature tends to reduce its yield stress. Quenching an aluminium-copper alloy, in contrast, results in moderate yield stress, which can then be increased by heating at a lower temperature.

For the alloys mentioned in (b), suggest approximate compositions and thermal histories which would lead to materials with the highest yield stress.