

Friday 9 June 2000

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 from this paper.

SECTION A

- 1** Define the term *flexural rigidity*. Briefly discuss, with examples, how the elastic deflection of a beam under load depends on both the materials from which it is made and the cross-sectional shape of the beam.

Show that the bending moment M in an initially straight elastic beam is related to its curvature ρ by the relationship

$$M = \frac{EI}{\rho}$$

where E is Young's modulus of the material and I is the second moment of area of the beam cross-section.

The axle of a railway carriage is a circular-sectioned bar of high-strength steel which is loaded in pure bending. Estimate the minimum size of surface flaw which will result in fast fracture occurring before any of the material exceeds the yield stress. At what value of bending moment will yielding first occur in an axle with a diameter of 40 mm?

[for this steel: fracture toughness $K_{\text{c}} = 40 \text{ MPa m}^{1/2}$; yield stress $\sigma_{\text{y}} = 1000 \text{ MPa}$]

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- 2 Discuss the factors which influence the yield stress of a polycrystalline cubic close-packed metal.

A dislocation is pinned at two points a distance L apart by fixed obstacles in its slip plane. Sketch the shapes adopted by the dislocation line as the shear stress τ on the slip plane is progressively increased. Show that the peak shear stress, at which the system becomes unstable, is given by

$$\tau = \frac{Gb}{L}$$

where G is the shear modulus of the material and b is the Burgers vector of the dislocation.

Prolonged heat-treatment of a magnesium-zinc alloy leads to the growth of large spherical precipitate particles in a matrix which is a very dilute solid solution of zinc in magnesium. If the precipitate material makes up 0.1 % of the volume of the alloy, and the heat-treatment raises its shear yield stress by 50 MPa, estimate the mean size of the precipitate particles. State your assumptions clearly.

[For magnesium $G = 17$ GPa]

- 3 Define the following terms: *lattice*, *motif* and *crystal structure*.

The mineral cassiterite, of composition SnO_2 , has the rutile structure with $a = 4.72 \text{ \AA}$ and $c = 3.16 \text{ \AA}$, and $u = 0.31$.

On graph paper, draw a plan on (001) of a 2×2 block of unit cells of the cassiterite structure.

- Mark in the mirror planes and rotational axes parallel to [001].
- How many formula units are there in the conventional unit cell?
- Describe the coordination polyhedron of O atoms around the Sn atom at (0, 0, 0).
- Calculate the distances from this Sn atom to the vertices of the polyhedron.

Calculate the angle between [110] and $[0\bar{1}2]$ in cassiterite. In which plane do these two directions lie?

- 4 Explain the following terms. Describe in each case how the concept is relevant to the application specified.
- (a) *vacancies* – application: oxygen sensor
 - (b) *liquid crystal* – application: optical display
 - (c) *radial distribution function* – application: structure of an inorganic glass
 - (d) *piezoelectricity* – application: gas lighter
 - (e) *pyroelectricity* – application: burglar detector

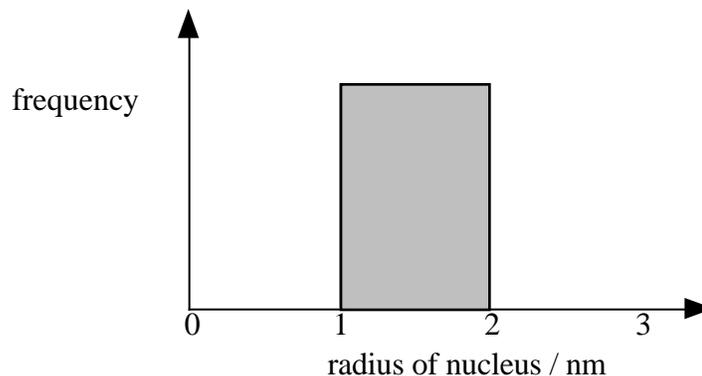
SECTION B

- 5 What factors control the homogeneous nucleation of a crystalline phase from a glass of the same composition? Derive an expression for the critical radius (r^*) of a spherical nucleus of such a crystalline phase. In your derivation, ignore any effects of elastic strain energy.

A glass-ceramic contains spherical crystal nuclei with initial sizes distributed as shown in the figure below. The number of nuclei in any size range is proportional to the relevant shaded area in the diagram. The total number density of nuclei is $1 \times 10^{14} \text{ m}^{-3}$. Subsequent annealing produces a fully crystalline material. How does the driving force for transformation vary with the annealing temperature? Calculate the annealing temperature required to produce a final grain size of $40 \mu\text{m}$ in the crystalline material.

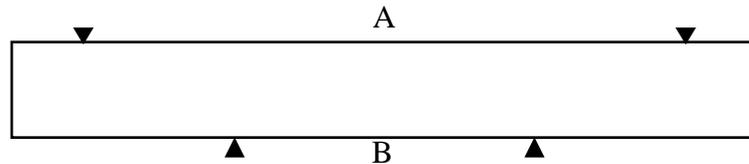
[Equilibrium temperature for the transformation $T_e = 1500 \text{ }^\circ\text{C}$; entropy change $S_v = 800 \text{ kJ m}^{-3} \text{ K}^{-1}$; interfacial energy $\sigma_{\text{glass/crystal}} = 0.25 \text{ J m}^{-2}$]

Figure for question 5:



- 6 Describe and explain the appearance of a quartz wedge viewed in the 45° position between crossed polars in white light. How would you use a quartz wedge to determine the fast and slow vibration directions in a strip of transparent polymer?

A sample of polycarbonate of rectangular cross-section mounted in a four point bending rig is observed through its thickness (1.5 mm) in yellow-green light ($\lambda = 558 \text{ nm}$) in the 45° position between crossed polars.



In the absence of load the sample appears dark. Sufficient load is applied to produce seven dark fringes across the full width (10 mm) of the sample between the inner pair of loading points, the outermost fringes being very close to the edges of the sample. What is the magnitude and nature of the stress at each of the edges A and B?

If the sample is now observed in white light, describe the appearance of the polycarbonate strip. A thin slice of quartz (thickness $62 \mu\text{m}$, cut parallel to the c -axis) is superimposed on the polycarbonate strip. At what position across the width of the strip is a dark fringe observed if the quartz slice is placed (a) with its c -axis parallel to the strip, or (b) with its c -axis perpendicular to the strip?

- 7 What factors determine the intensities of lines in X-ray powder diffraction? Why do the X-ray scattering properties of an atom or ion depend on its atomic number?

An equiatomic alloy of copper and zinc is equilibrated at 750°C and the structure is found to be cubic with $a = 3 \text{ \AA}$. The indices of the first five powder lines are 110, 200, 211, 220 and 310. Sketch a possible structure for the alloy and indicate its lattice type.

Below 460°C an ordering reaction occurs in this phase. The lattice type is believed to be cubic P. X-ray powder diffraction reveals that the 100, 111, 210 and 300/221 lines are present but very weak. Suggest and sketch a possible structure for the ordered alloy. Calculate the structure factors for the 100 and 111 lines for this structure. Hence explain why these reflections are weak.

How would the X-ray powder diffraction pattern for an alloy containing 70 wt% copper and 30 wt% zinc differ from that of the equiatomic alloy?

[atomic scattering factors $f_{\text{Cu}} = 29$; $f_{\text{Zn}} = 30$]

- 8 Explain how the periodicities present in high-resolution images in a transmission electron microscope relate to those present in the electron diffraction pattern used to form the image.

On graph paper, draw the appearance of the electron diffraction pattern that will be recorded when the incident electron beam is parallel to the $[1\bar{1}0]$ direction of aluminium, indexing spots with $h^2 + k^2 + l^2 = 12$.

An aperture is set to accept beams in this diffraction pattern corresponding to planes with interplanar spacings $> 1.5 \text{ \AA}$. By treating the image formed from these beams as the points of intersection of gratings of narrow slits suitably oriented with respect to one another, draw on graph paper the expected appearance of this image. Comment on the relationship between this image and the crystal structure of aluminium projected along the $[1\bar{1}0]$ direction.

SECTION C

- 9 Derive the Clausius-Clapeyron equation. Explain why the phase boundaries on a pressure-temperature ($P - T$) diagram are approximately straight lines.

Ice has several polymorphs which are stable at different temperatures and pressures. Two phases have melting points near $0 \text{ }^\circ\text{C}$. One is Ice (I), which is stable at atmospheric pressure; the other is Ice (V) which is stable only at much higher pressures. The table lists measured values of melting pressures at three temperatures.

Temperature / $^\circ\text{C}$	Ice (V) / MPa	Ice (I) / MPa
0.00	629.1	0.1
- 0.25	623.9	3.6
- 0.50	618.8	7.0

For each polymorph, calculate the mean value of dP/dT between $0 \text{ }^\circ\text{C}$ and $- 0.5 \text{ }^\circ\text{C}$. Suggest a reason for the major difference between these two values.

Ice (I) has a density of 0.917 Mg m^{-3} at $0 \text{ }^\circ\text{C}$ and atmospheric pressure. The density of liquid water rises by 19% when the pressure is increased from 0.1 MPa to 629.1 MPa. The entropy change due to melting of Ice (I) is 16% greater than that for melting of Ice (V). Estimate the density of Ice (V) at $0 \text{ }^\circ\text{C}$ and 629.1 MPa.

[Assume that the density of liquid water at $0 \text{ }^\circ\text{C}$ and atmospheric pressure is 1.000 Mg m^{-3}]

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- 10 Define the terms *supersaturated solid solution*, *precipitation hardening* and *overaging*. Why is overaging preferable to underaging in a precipitation-hardened alloy?

The Ag-Al phase diagram is provided below. Aluminium can be hardened by alloying with silver. Suitable heat treatments can then give precipitation hardening. The precipitation sequence is

Silver-rich G.P. zones

and have approximately the same chemical composition.

Explain briefly why precipitation sequences such as this occur.

You are asked to give advice on the choice of composition for a precipitate-hardened Al-Ag alloy. Explaining your reasoning,

- recommend a composition to achieve maximum hardening by precipitation in the Al-rich matrix, and
- recommend a temperature for solution heat-treating.

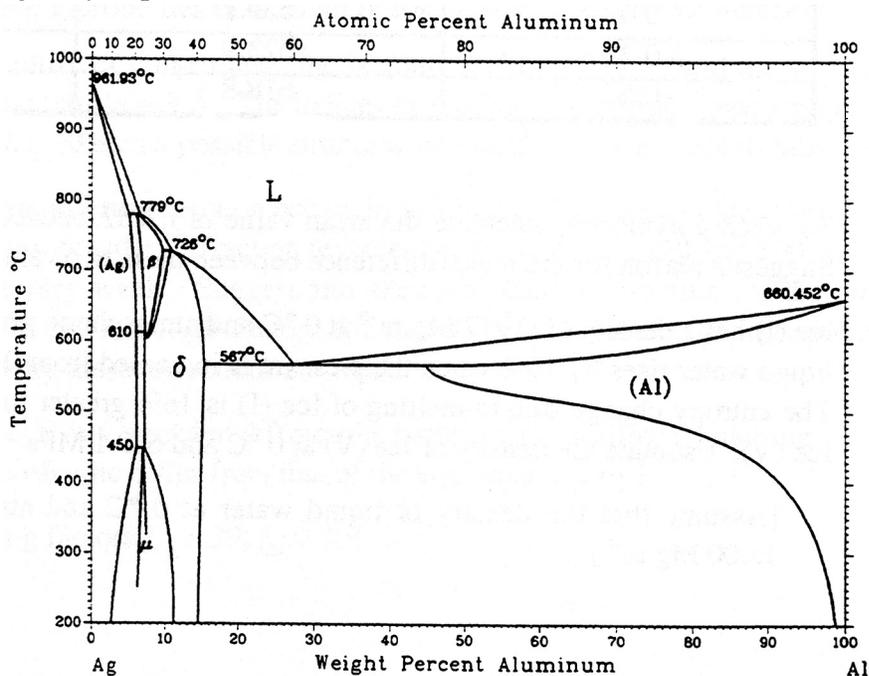
Assuming that precipitation occurs at 200 °C, estimate the maximum obtainable weight fraction of precipitate for the alloy composition you recommend.

precipitates have an ideal close-packed hexagonal crystal structure in which the Ag and Al atoms are randomly arranged on atomic sites. These precipitates are coherent with the matrix and have an orientation relationship with the matrix of

$$(001) \cdot \parallel (111)_{\text{matrix}} ; [100] \cdot \parallel [10\bar{1}]_{\text{matrix}}$$

Deduce the lattice parameters of .

Phase diagram for question 10:



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