NATURAL SCIENCES TRIPOS Part IA

Friday 7 June 2002 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 Describe the atomic scale structure that gives rise to different stiffnesses in the polymeric, metallic and ceramic classes of material. Explain the general trend of $E_{polymer} < E_{metal} < E_{ceramic}$, where E is Young's Modulus.

Assuming equal strain in the constituent materials, derive the equation describing the axial Young's modulus of a unidirectional fibre reinforced polymer composite, as a function of the moduli and volume fractions of the constituents.

A high pressure water pipe is manufactured from polypropylene reinforced with kevlar fibres. The pipe has internal and external diameters of 90 mm and 100 mm respectively. The pipe is reinforced with 15% (by volume) unidirectional fibres wound in the hoop direction only. Calculate the stiffness of the pipe in the hoop direction. The pipe is pressurised to 20 bar. Estimate the maximum stress levels in the wall of the pipe and, hence, calculate the load borne by the reinforcing fibres. Comment on the suitability of such a construction for use as a high pressure water pipe. [$E_{polypropylene}$ = 2 GPa, E_{kevlar} = 125 GPa]

2 Explain why ceramic materials have low tensile strengths, but are very strong in compression.

Some alumina samples were carefully pre-cracked prior to tensile testing. The table below summarises the resultant strengths for a variety of pre-crack lengths. The fracture strengths quoted are the average of a large number of tests.

Introduced crack length (mm)	Fracture strength (MPa)
0.10	250
0.25	160
0.50	110
1.00	80

Calculate the critical strain energy release rate (G_c) for this material.

Uncracked alumina specimens have a tensile failure strength of 5 GPa. Estimate the intrinsic flaw size present in these specimens. Suggest methods by which this failure strength could be improved.

3 Silicon carbide (SiC) has many polymorphs. The most common one has the wurtzite structure (hexagonal, a = 3.08 Å, c = 5.05 Å) with atoms in the positions:

Si: 0,0,0; $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ C: 0,0,$\frac{5}{8}$; $\frac{2}{3},\frac{1}{3},\frac{1}{8}$

Draw a plan of 2 x 2 unit cells viewed down [001]. Determine the lattice type and list any centres of symmetry, rotation axes or symmetry planes which may be present in the structure, giving their positions or orientation.

Another polymorph has the sphalerite structure (cubic F, a = 4.36 Å), with atoms in positions:

Si: 0,0,0 C: $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

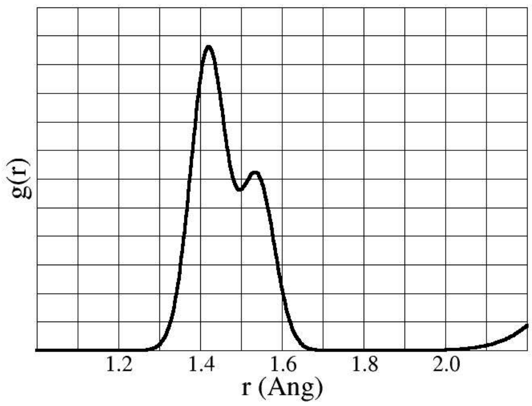
Sketch the arrangement of Si atoms on the (111) plane. Describe how successive (111) planes of Si atoms are stacked to give the complete structure.

Describe the main structural difference between the two polymorphs? Based on this, how might other polymorphs of SiC be generated?

4 Define the term *radial distribution function* and explain what kind of information it gives concerning the structure of solids.

Two polymorphs of pure carbon are diamond (a = 3.57 Å) and graphite (hexagonal, a = 2.46 Å, c = 6.68 Å, with atoms at 0,0,0; $\frac{2}{3},\frac{1}{3}$,0; 0,0,$\frac{1}{2}$; $\frac{1}{3},\frac{2}{3},\frac{1}{2}$). Draw the radial distribution function, $g(r)$, of each polymorph out to 3 Å.

The radial distribution function, $g(r)$, of a sample of amorphous carbon is given below.



How might this observed distribution be related to your calculations for diamond and graphite?

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SECTION B

5 Using appropriate examples of phase diagrams, explain the terms *eutectic* and *eutectoid*. Why do some binary phase diagrams contain a eutectic point while others do not?

Computer modeling of a new binary alloy system, based on thermodynamic data, suggests that it should have partial solid solution in both end members and a eutectic point.

(i) Describe the cooling curves you would expect to observe for initial melts with different compositions in this system, if the computer prediction is correct.

(ii) Explain the microstructures you would expect to observe in the final, fully crystallised samples for each of the compositions described in (i) above. Indicate how the proportions of the final phases might be predicted.

A subsequent computer model suggests that one of the end member phases might undergo a reconstructive phase transformation at a temperature which is a few hundred degrees below its melting point. Sketch the form of phase diagram which you would expect to find for this system, if the model is correct.

6 Describe what happens in a ferroelectric material when it is placed in an electric field. Why does its polarisation display a hysteresis loop when the applied field is cycled?

A wafer of $BaTiO_3$, 0.1 mm thick, is placed between the plates of a capacitor. Each plate has a surface area of 4×10^{-6} m^2, the permittivity of $BaTiO_3$ at room temperature is 8.9×10^{-9} F m^{-1}, and a potential difference of 5 V is applied across the plates. Calculate (a) the capacitance, (b) the magnitude of the charge stored on each plate, (c) the charge density on the surface of the plates, and (d) the polarisation in the $BaTiO_3$.

$BaTiO_3$ undergoes a phase transition at 117 ˚C. Briefly suggest how the properties calculated in (a) – (d) above would change as a function of temperature if the capacitor containing $BaTiO_3$ was heated to 130 ˚C.

7 Summarise the factors that determine the intensities of Bragg reflections observed in X-ray powder diffraction patterns.

Assuming that the atomic scattering factors have magnitudes equal to their values at zero diffraction angle, estimate the relative magnitudes of the intensities for the first four Bragg reflections that would be observed in the X-ray powder diffraction pattern from a sample of sodium chloride ($a \approx 5.6$ Å) using nickel-filtered CuKα radiation. Comment on the validity of the assumption about atomic scattering factors. How would the pattern obtained in otherwise identical circumstances from a sample of potassium chloride differ from that for sodium chloride.

A high angle line, identified as the 444 reflection, observed in the pattern for sodium chloride is a closely spaced doublet with Bragg angles $\theta = 71.52°$ and $\theta = 71.95°$. Calculate an accurate value for the lattice parameter and estimate the accuracy of your result.

8 Indicate briefly what is meant by the terms *reciprocal lattice* and *Ewald sphere*. Explain how the reciprocal lattice and the Ewald sphere may be used:

(a) to interpret electron diffraction patterns from a thin crystalline sample;

(b) to work out how to obtain a dark field image of a selected region in the sample.

Sketch the electron diffraction pattern that would be obtained from a single grain in a thin sample of aluminium when the incident beam is exactly parallel to the $[0\bar{1}1]$ direction in the grain. Index all the reflections for which $h^2 + k^2 + l^2 \leq 16$. Through what angle and about what axis must the crystal be tilted in order to obtain an optimum dark field image using the 022 reflection with electrons accelerated through 100 kV?

The surface of a grain in a thin sample of aluminium is known to be parallel to $(11\bar{1})$. Some dark field images from the grain show a dislocation line which may be assumed to be parallel to the surface. The line becomes invisible when the dark field image is formed using the 222 reflection. Determine the Burgers vector of the dislocation.

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SECTION C

9 Describe briefly the hierarchical structure of *ligament* and *cortical bone*.

Some stress-strain data obtained for ligament and cortical bone, but not identified, are as follows:

Specimen X		Specimen Y	
Stress (MPa)	Strain (%)	Stress (MPa)	Strain (%)
0	0	0	0
5	2.0	20	0.08
10	2.8	40	0.16
20	3.5	60	0.24
30	4.2	80	0.32
40	5.0	100	0.40
50	5.8	120	0.51
60	12.0		

Use these data to plot stress vs strain curves and determine the elastic modulus for each material. Identify Specimen X and Specimen Y, giving reasons for your choice.

Suggest, with reasons, suitable synthetic materials for (a) replacement of a ruptured cruciate ligament, and (b) a bone graft to aid repair of a tibial fracture.

10 The Antarctic ice sheet can be up to a few km deep and forms by compaction of deposited snow which shows an annual variation in relative isotopic abundances. This variation, preserved in the ice, is of interest for studies of climate over the last tens of thousands of years. The variation decays with time because of diffusion of H_2O molecules in the ice. Given that the thickness of ice associated with one year's snow deposition is 0.1 m, estimate the period before the annual isotopic variation would show a significant smearing, and comment on the value obtained. The ice is at a temperature of approximately –30˚C.

Estimate the depth of ice such that material at the bottom would melt under the weight of that above. Comment on the likelihood of melting at the base of the ice sheet. Suggest likely mechanisms by which loosely deposited snow can be compacted into ice with no porosity.

[For ice: diffusivity of H_2O molecules $D = D_o \exp(-Q/RT)$, where $D_o = 1.24 \times 10^{-4}$ m^2 s^{-1}, Q = 54.5 kJ mol^{-1}, R is the gas constant and T is the temperature; density ≈ 0.92 Mg m^{-3}; latent heat of melting = 333.5 kJ kg^{-1}]

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