MASTER OF PHILOSOPHY Modelling of Materials

Friday 23 April 2004 9 to 12.00

MODELLING OF MATERIALS (2)

Answer **six** *parts from Section* **A** *(i.e. Question 1),* **two** *questions from Section* **B**, *and* **one** *question from Section* **C**.

Each **Section** *carries* **one-third** *of the total credit for this paper.*

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

The answer to **each question** *must be tied up* **separately**, *with its own cover-sheet. All the parts of Question 1 should be tied together.*

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

For questions divided into parts, the **approximate** *fraction of credit allocated to each part is indicated by the percentages in square brackets.*

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. (a) Explain what is meant by a *dislocation* in a crystal, and how the character of the dislocation can be described. What effect does the presence of dislocations have on the mechanical properties of a perfectly crystalline material?

   (b) Stress and strain are both 3×3 tensors, which can be related by Hooke's law. To relate two completely general 3×3 tensors in this way would require an 81 element fourth rank tensor. Explain why fewer constants are needed to relate stress and strain. How many independent constants relate stress and strain in (i) the most general case, and (ii) an isotropic solid?

   (c) Outline why quantitative modelling of materials production and processing may be of interest to industry, despite the cost of developing the model.

   (d) State the Bragg condition for electron wave reflection in *k*-space. Use this to explain how Brillouin zones are constructed in a crystal and give a definition of the *n*th Brillouin zone.

   (e) Discuss, with examples (which need not include FORTRAN code), the advantages of using subroutines and functions in the FORTRAN programming language.

   (f) Explain why *grain growth* occurs on annealing a polycrystalline metal. Why do some grains shrink even as the average size increases? How do the geometry of grain boundaries and their junctions affect the tendency of a grain to shrink or grow?

   (g) What is thermal importance sampling, and how is it achieved by the Metropolis Monte Carlo method?

(h) Describe the operations occurring in each of the three stages comprising the Finite Element Method. At what stage are any errors incurred most likely to have the greatest influence on the final answer?

(i) Write down the phase rule and define the terms. Why, under normal circumstances, is one degree of freedom already defined? State the conditions for three phases to be in equilibrium in a two-component system.

(j) What are the main factors to consider in selection of a shaping process? Explain briefly why the Cambridge Engineering Selector software has separate databases for joining and surface treatment. Explain, with an example, why the processing rate is generally not a simple characteristic of a given process.

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SECTION B

2. State the basic assumptions of the free electron model. Sketch the form of the electron energy dispersion curve *E(k)* for free electrons in a one-dimensional box. Define the terms *Fermi energy* and *Fermi wave-vector* and mark these on your sketch. Sketch also the shape of the Fermi surface for free electrons in a three-dimensional box and explain why deviations from this shape are expected in reality.

[30%]

What is meant by the *density of states*? Show that for free electrons in three dimensions, the density of states is proportional to $\sqrt{E}$.

[50%]

Consider the *average* energy $\langle E \rangle$ of free electrons in a three-dimensional box. This quantity may be defined as the total electron energy divided by the total number of electrons. By performing suitable integrations over the density of states show that $\langle E \rangle = 3E_F/5$ where E_F is the Fermi energy.

[20%]

3. Discuss how it is possible to predict phase diagrams from thermodynamic models. Illustrate your answer by reference to the excess Gibbs free energy for binary and ternary solutions.

[40%]

What are the advantages and disadvantages of this approach?

[20%]

The enthalpy of mixing of two components A and B is $\omega x_A x_B$, where x_A and x_B are the fraction of A and B atoms and $\omega = 20$ kJ mol^{-1}. Assuming the entropy of mixing is ideal, calculate the temperature at which immiscibility will occur on cooling.

[40%]

4. Materials are to be selected for a tensile strut and a panel loaded in bending. Both are limited by the allowable stiffness, and the objective is to minimise the mass in each case. The length of the strut, L, and the plane dimensions of the panel, $L \times B$, are fixed. The cross sectional area, A, of the strut and the thickness of the panel, D, may be varied from material to material.

The stiffness, S, of the members are defined by:

$S = \dfrac{L}{AE}$ for the strut, and $S = \dfrac{C_1 L^3}{E B D^3}$ for the panel (where C_1 is a constant and E is the Young's modulus).

Write down an expression for the mass of the strut and the mass of the panel. Use the stiffness equations to eliminate the dimensional variable in each case, and hence find the performance index to minimise for minimum mass struts and panels.

[30%]

Evaluate the performance indices for the materials in the table below, and comment on the competition between materials for lightweight tensile members and panels, limited by stiffness.

	Yield stress σ_y (MPa)	Young's modulus E (GPa)	Density ρ (Mg/m^3)	Cost per kg C_m (£/kg)
Low alloy steel	1100	209	7.85	0.40
Ti alloy	1245	105	4.6	35
Mg alloy	400	44.5	1.85	3
CFRP	1050	110	1.55	40

Show by an annotated sketch how this evaluation can be made graphically on a material property chart.

[70%]

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5. Outline the distinguishing features of:

(i) The lattice gas model of Frisch, Hasslaucher and Pomeau
(ii) The lattice director model for liquid crystalline systems

[30%]

A lattice director model is used to simulate the phase transformation from a nematic to an isotropic phase. Write down the Hamiltonian used for this model (assuming that splay, twist and bend elastic constants are equal), and the computational protocol appropriate to monitor the microstructure as a function of temperature in the transition region.

[40%]

Explain how a similar Hamiltonian would be appropriate to modelling the coarsening of a nematic microstructure, using a finite difference algorithm. Outline why a temperature-type factor might be introduced into such an algorithm.

[40%]

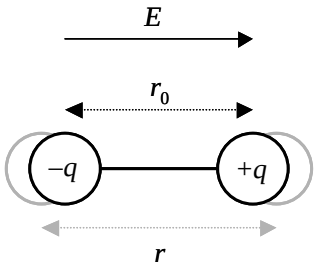
SECTION C

6. Describe the *molecular mechanics* approach to modelling atomistic systems, including in your answer a definition of the term force field. Give an example of a commonly used force field, and briefly describe the physical origin of each of the terms in the energy expression.

[20%]

Explain how *energy minimisation* can be used in conjunction with a force field to model atomistic systems, illustrating your answer with two distinct examples. Give an example of a numerical algorithm that could be used to minimise the energy of a large atomistic system. What are the disadvantages of energy minimisation?

[40%]



The above diagram shows schematically the symmetric stretch of linear dipolar molecule, with atomic point charges $\pm q$, under the influence of an applied electric field E, where r_0 and r are the equilibrium bond length and stretched bond length, respectively.

Assuming the bond stretching energy can be approximated by a harmonic function with force constant k, and the atomic charges do not interact with each other, construct a potential energy expression for the molecule in the applied field. Minimise this energy expression with respect to the bond length r, and calculate r/r_0 when $q = 96352$ C mol^{-1}, $r_0 = 1$ Å, $k = 10^3$ kJ mol^{-1} Å^{-2} and $E = 10^4$ kV m^{-1}.

[40%]

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7. What form does the attractive (or bonding) part of the potential take in (i) the embedded atom method and (ii) the Finnis-Sinclair potential? Give a physical justification for these forms.

[30%]

In one model of a transition metal, the energy per atom is given by:

$$U = \frac{1}{2}\sum_{i\neq 0} V(r_i) - A\left(\sum_{i\neq 0}\phi(r_i)\right)^{1/2}$$

where A is a constant and the pair potentials $V(r_i)$ and $\phi(r_i)$ take the following forms:

$$V(r) = (r-c)^2\left(c_0 + c_1 r + c_2 r^2\right) \qquad \phi(r) = (r-d)^2$$

Consider the application of this model to tungsten (bcc, a_0 = 3.1652 Å) and assume that interactions beyond second nearest neighbours can be ignored. Let V_1 and ϕ_1 be the potentials at the first neighbour distance and V_2 and ϕ_2 be the potentials at the second neighbour distance. Evaluate these potentials for tungsten using data below.

[20%]

The vacancy formation energy E_V in tungsten can be obtained by summing V and ϕ over those atoms within range of the vacancy whose coordination has changed, and subtracting the corresponding perfect lattice terms. By doing this show that:

$$E_V = -(4V_1 + 3V_2) - A\left[8(7\phi_1 + 6\phi_2)^{1/2} + 6(8\phi_1 + 5\phi_2)^{1/2} - 14(8\phi_1 + 6\phi_2)^{1/2}\right]$$

[40%]

Evaluate E_V for tungsten and suggest why this value is likely to be larger than the experimental value of 3.15 eV.

[10%]

[For tungsten: d = 4.4002 Å, A = 1.8964 eV/Å, c = 3.25 Å, c_0 = 47.1346 eV/Å^2, c_1 = -33.7666 eV/Å^3, c_2 = 6.2542 eV/Å^4]

END OF PAPER