MASTER OF PHILOSOPHY   Modelling of Materials

Friday 27 April 2007   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.*

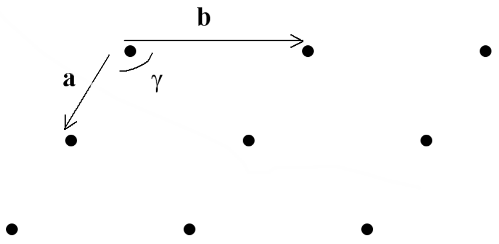
Special and/or stationery requirements for this paper: **graph paper**

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) Distinguish between *homogeneous* and *heterogeneous* nucleation. What are the main difficulties in quantitative modelling of these phenomena?

   (b) Illustrated below is an oblique 2-D reciprocal lattice defined by the vectors **a** and **b** and the angle γ. Sketch the 1st Brillouin zone of this lattice and determine its area.



   (c) Draw a schematic diagram of a dye sensitised solar cell, and indicate on this four fundamental physical processes that govern its operation.

   (d) Explain the advantages of using a polynomial expression of the following form:

$$x_{\mathrm{A}} x_{\mathrm{B}} \sum_{i=0}^{j} L_{\mathrm{AB},i} \left(x_{\mathrm{A}} - x_{\mathrm{B}} \right)^{i}$$

   to describe the enthalpy of mixing in a binary A-B solution, where $x_{\mathrm{A/B}}$ refers to the mole fraction of species A/B. Give the usual name for a solution with $j = 0$, and also in the special case where $L_{\mathrm{AB},0} = 0$.

   (e) The FORTRAN programming language allows the declaration of array variables. Describe three possible uses of such variables. There is no need to provide FORTRAN code in your answer.

(f) What are the factors that contribute to the heat capacity of a metal? Explain in particular the role of the electrons. What additional factors contribute to the heat capacity of a polymer?

(g) Verify from its definition that the Gibbs free energy is an exact function of state. Explain why it is not possible to calculate the Gibbs free energy from an isothermal-isobaric simulation by averaging over configurations.

(h) In a Potts Monte Carlo model for microstructural evolution, describe how grain boundaries are defined and what determines their motion.

(i) Explain clearly the difference between noise in experimental data and the uncertainty of modelling.

(j) Discuss briefly the issues relating to the creation of a mesh suitable for the finite element analysis of the temperature distribution produced during welding of large structures and describe some meshing strategies by which these issues may be addressed.

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SECTION B

2. Describe what is meant by the *Fermi surface* of a solid and explain its physical significance.

[30%]

What is the shape of the Fermi surface for a perfect free electron metal? For such a metal, show that the Fermi wave vector, k_F, is given by $k_\mathrm{F} = \left(3\pi^2 n\right)^{1/3}$, where n is the electron density.

[30%]

Copper is monovalent and has the fcc structure with lattice parameter equal to 0.36 nm. Calculate the value of k_F that copper would have if it were a free electron metal. What volume fraction of the first Brillouin zone is occupied by the Fermi surface defined by this k_F?

[20%]

How does the experimentally measured Fermi surface of copper differ from that of a free electron metal? Provide a brief explanation for the difference.

[20%]

3. It is usual in steady-state processes to assume that a generalised flux J is proportional to a generalised force X. By taking an appropriate Taylor expansion of J as a function of X, reveal the approximation involved in assuming that $J \propto X$.

[40%]

Derive an expression for the velocity of a grain boundary during interface-controlled growth as a function of the activation energy, G^*, for the transfer of atoms across the interface, and of the magnitude of the free energy difference, ΔG, between the parent and product phases.

[45%]

Show that the velocity (a flux) is proportional to ΔG (a force) when the latter is small, but not when it is large.

[15%]

4. What factors are important in the design of a solid punt pole? Describe the various ways that a pole might fail.

[20%]

Derive a performance index for the pole itself and, using the Materials Selection charts **provided on Page 7**, identify three possible materials. Discuss their relative advantages.

[60%]

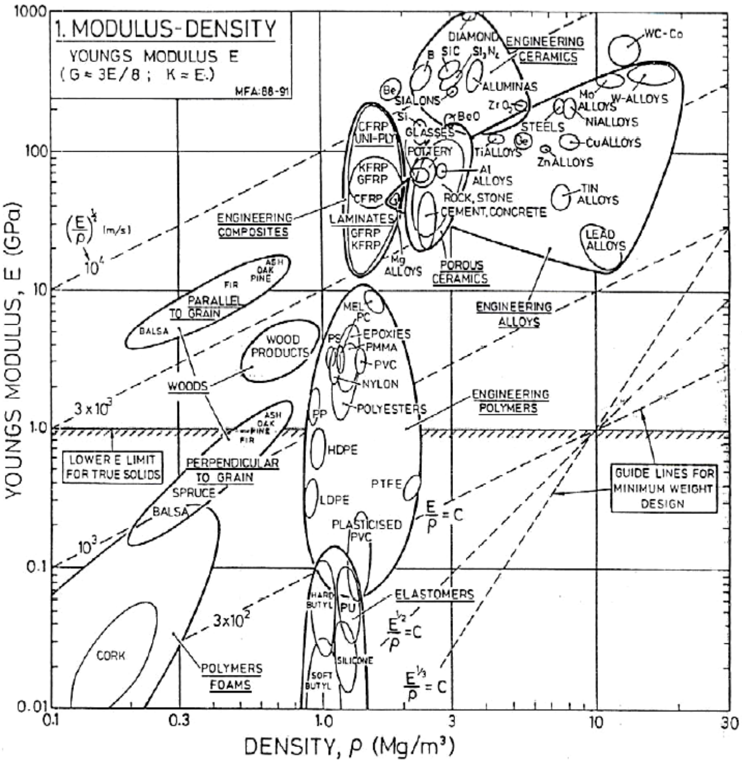
How might you improve the design of a punt pole and how might this influence the choice of materials?

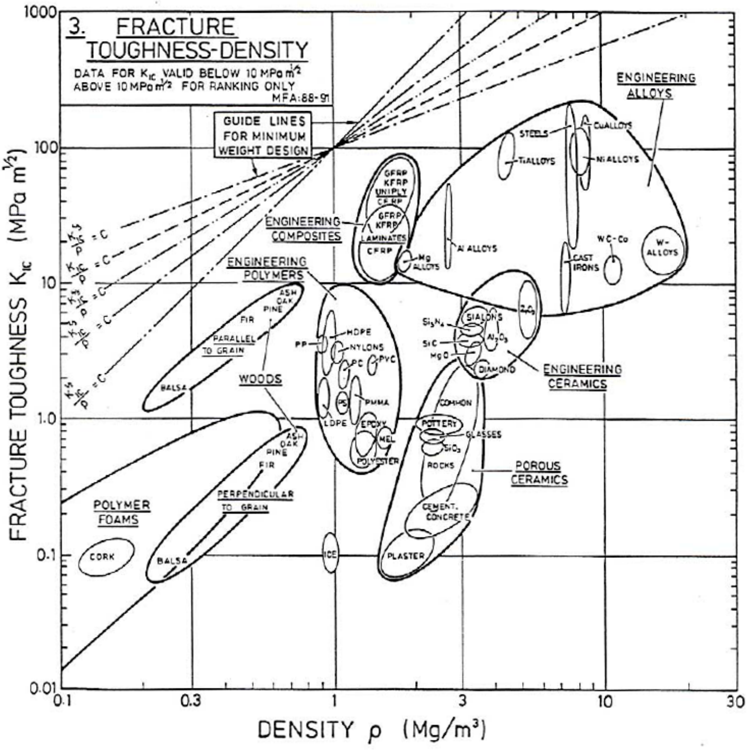
[20%]

[Additional information: to avoid elastic buckling of a beam in compression, the applied force $F < \frac{C \pi^2 E I}{x^2}$,

where E is Young's modulus, x is the beam length, C is a constant, and I is the second moment of area, which for a circular solid beam of radius r is given by $I = \pi r^4 / 4$]

Materials Selection maps required for Section B, question 4.





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5. Consider the motion of an isolated molecular particle moving on a one-dimensional potential energy surface with functional form:

$$U(x) = \begin{cases} \alpha A x^2 & x < 0 \\ \alpha\left[1 - \cos\left(2\pi x\right)\right] & 0 \le x \le 1 \\ \alpha A\left(x-1\right)^2 & x > 1 \end{cases}$$

where α is some positive constant.

Given that the energy U, the force and derivative of the force are continuous at all points on the curve, derive an expression for the constant A, and hence produce an annotated sketch of the potential indicating any stationary points.

[50%]

A canonical NVT molecular dynamics (MD) simulation was carried out for an isolated particle in the potential U, initially at rest with position $x = 0$. Briefly explain the MD algorithm, and describe a method by which temperature control could be achieved.

[30%]

Using the information above, describe qualitatively the behaviour of the system as the temperature is increased from $T = 0$. You are not expected to carry out any MD simulations.

[20%]

SECTION C

6. Describe the condition for thermodynamic equilibrium between two pure phases.

[10%]

What is meant by the term chemical potential and how is this concept used in describing equilibrium between solid solutions? Illustrate how this justifies the common tangent construction that is used to find the equilibrium compositions of phases in contact.

[25%]

The binding energy between two atoms brought together from infinite separation to an equilibrium separation is defined as $-2\varepsilon_{ij}$, where the subscripts refer to the atomic species. Calculate the total internal energy due to the bonds in physically separated samples composed of purely A and B components containing $N(1-x)$ and Nx atoms, respectively, where x is a mole fraction.

[25%]

Given a binary solid solution of N atoms of which xN are B atoms and the remainder A atoms, derive expressions giving the numbers of AA, BB, AB and BA nearest neighbours, stating clearly any assumptions you make. What is the total internal energy of such a solution?

[25%]

Hence derive an expression for the enthalpy of mixing.

[15%]

7. The properties of polycrystalline solids may be affected by the average grain diameter, strongly in some cases, weakly in others. In some cases the property varies straightforwardly over the entire range of achievable grain diameter; in others, distinctive properties appear in nanocrystalline materials. Explain how such effects arise, taking examples of thermodynamic, elastic, plastic, optical and magnetic properties.

[40%]

Distinguish between diffusional creep and superplastic flow in terms of the effects on the grain structure of a material. What is the main mechanism of superplastic flow? Outline the requirements for the grain structure of a superplastic material and the methods by which the desirable grain structure may be maintained. Explain why nanocrystalline materials are of interest for superplastic flow, and give examples of the types of materials that may benefit from a nanocrystalline grain structure.

[40%]

The superplastic flow rate $\dot{\varepsilon}$ of alumina depends on the grain size d and the temperature T according to

$$\dot{\varepsilon} \propto d^{-2.5} \exp\left(-\frac{Q}{RT}\right)$$

where R is the gas constant (8.314 J K^{-1} mol^{-1}) and the activation energy Q is 250 kJ mol^{-1}. If polycrystalline alumina with a grain size of 600 nm shows a satisfactory rate of superplastic flow at 1200˚C, by how much would this temperature be lowered for a sample with a grain size of 60 nm?

[20%]

END OF PAPER