MASTER OF PHILOSOPHY   Modelling of Materials

Thursday 22 April 2004   9 to 12.00

MODELLING OF MATERIALS (1)

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) Draw a projection along the *z*-axis of the crystal structure of diamond, which has a face-centred cubic lattice with a motif of carbon atoms at 0,0,0 and ¼, ¼, ¼. How many lattice points are there in this unit cell? How many atoms are there per unit cell?

(b) Explain how the number of allowed electrons in a band can be used in a simple way to distinguish between a metal and an insulator. Illustrate your answer with specific examples.

(c) Explain what is meant by a multiscale computer model. Give an example of a problem in materials science where it could be advantageous to use this type of model. What is the main technical difficulty in its implementation?

(d) Explain what is meant by an *irreversible process* and a *steady-state process* in the context of thermodynamics. 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 $J \propto X$.

(e) The second rank tensor T transforms to the tensor T' in a new basis: $T' = LTL^T$, where L is the appropriate rotation matrix given in suffix notation by $T'_{\alpha\beta} = L_{\alpha i} L_{\beta j} T_{ij}$.

Write a FORTRAN subroutine which, when given two 3×3 real arrays representing T and L as its first two arguments, returns with a third argument, also a 3×3 real array, set to T'.

(f) Outline three major differences between the mould design for an injection moulded thermoplastic polymeric component and for a cast metal component.

(g) Explain how the SHAKE algorithm can be used to constrain the bond length during the molecular dynamics simulation of a simple diatomic molecule.

(h) Explain the difference between Brownian Dynamics (BD) and Dissipative Particle Dynamics (DPD), and describe the application of DPD to modelling of self-assembly of short, diblock copolymer molecules.

(i) In phase field theory, the term g describes how the free energy varies as a function of the order parameter, and can be written as

$$g = \int_V \left[g_0\{\phi, T\} + \varepsilon(\nabla\phi)^2 \right] \mathrm{d}V$$

where V represents the volume, T is the absolute temperature, and g_0 is the free energy of a homogeneous system. Explain in words the meaning of the order parameter ϕ and the term $\varepsilon(\nabla\phi)^2$.

(j) Describe three factors that influence the shape of precipitates.

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SECTION B

2. Describe how an artificial neural network model is constructed. What are the advantages of neural network modelling when compared with linear regression analysis?

[20%]

How is the problem of overfitting avoided in neural network analysis?

[25%]

How does the quantity of data used in the development of a neural network model affect its ability to predict?

[15%]

Are there any other factors besides the quantity of data that influence the ability of the trained network to predict accurately?

[30%]

Suggest a suitable collection of data that could be used to predict the strength of a steel weld using a neural network model.

[10%]

3. In *precipitation hardening* of an Al-Cu alloy, the yield stress shows a maximum as a function of annealing time. Why is precipitation hardening of technological interest?

[10%]

How does the precipitation affect the Young's modulus and electrical resistivity of the material?

[20%]

What are the mechanisms of the observed hardening? Why does the yield stress show a maximum?

[40%]

Which types of modelling might be useful for predicting the hardening behaviour?

[30%]

4. Finite element analysis can be applied to generate numerical solutions for a wide range of problems, ranging from thermal heat transfer to stress-strain analysis.

   Identify the main parameters involved in the pre-processing analysis of two-dimensional heat transfer in a composite structure. What would be the ideal element for this problem? Explain your answer.

   [25%]

   What additional parameter or requirements are necessary for the simulation of problems in which large scale deformation occurs? (*e.g.* metal forming processes).

   [25%]

   Provide a definition of a shape function, and describe the role of shape functions in finite element analysis, using appropriate sketches to illustrate your answer.

   [40%]

   Numerical solutions to the Jominy end quench bar were shown to vary significantly as the boundary conditions were varied during the finite element simulations. How would you determine which solution is correct?

   [10%]

5. Give an expression for the *partition function* of a system consisting of a fixed number of particles N in thermal equilibrium with a reservoir at temperature T as a sum over microstates, defining any terms used. How is the partition function related to the Helmholtz free energy of the system?

[20%]

Consider a three-state system with energy levels $-V\varepsilon$ and $+V\varepsilon$ relative to the ground state with zero energy, where V is the total volume and ε is a constant. Write down the partition function for a system of N independent, distinguishable particles. By considering the differential form of the Helmholtz free energy, derive an equation of state relating the pressure of the system to some function of volume, temperature and particle number to be determined.

[50%]

Explain the problem with applying the above method to a system of non-independent particles, and suggest an appropriate method for calculating the equation of state using computer simulation.

[30%]

SECTION C

6. Describe what is meant by diffusion-controlled and interface-controlled growth.

[20%]

How would you calculate the growth rate in circumstances where growth occurs under mixed control?

[20%]

Show that when spherical precipitates grow at a constant rate *G* and a constant nucleation rate I_V , the volume fraction ξ is given by

$$\xi = 1 - \exp\left\{-\pi G^3 I_V t^4 / 3\right\}$$

[30%]

A supersaturated solution is allowed to transform isothermally. The evolution of the volume fraction as a function of time is given in the table below. The precipitates are found to grow isotropically and at a constant rate. Deduce the time exponent and explain why it differs from the value found in the equation above.

ξ	Time [s]
0.1	84
0.3	126
0.5	157

[30%]

7. Explain the difference between a mechanical mixture and a solid solution.

[20%]

Calculate the number of A-A, B-B, and A-B + B-A bonds in a random mixture of A and B atoms, with the total number of atoms equal to one mole.

[20%]

Given a binary solution containing A and B atoms, show that the enthalpy of mixing per mole of atoms is given by:

$$\Delta H_{\mathrm{M}} = zN_{\mathrm{A}}x(1-x)\omega$$

where N_{A} is Avogadro's number, z is a coordination number, x is the concentration of the B atoms and $\omega = \varepsilon_{\mathrm{AA}} + \varepsilon_{\mathrm{BB}} - 2\varepsilon_{\mathrm{AB}}$. Here, ε are the binding energies (per atom) of the atom pairs.

[40%]

State any approximations involved in your derivation.

[10%]

Real solutions do not exhibit the symmetry in ΔH_{M} about x = 0.5. How is this resolved in the computer calculation of phase diagrams?

[10%]

END OF PAPER