

MODELLING OF MATERIALS (2)

*Answer **six** parts from Section **A** (i.e. Question 1), which carries **one-third** of the credit for this paper.*

***Two** questions should be answered from Section **B**; these two questions carry **one-third** of the credit for this paper.*

***One** question should be answered from Section **C**; this carries **one-third** of the 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.*

<p>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</p>

SECTION A

1. (a) In atomistic modelling it is useful to expand the potential energy of the material into pairwise and higher terms. Write an expression for this expansion. Describe the circumstances in which it would be appropriate to use the Axilrod–Teller potential.
- (b) Describe five experimental methods used in the determination of equilibrium phase diagrams.
- (c) Describe what you would need to include in the documentation of a materials algorithm expressed as a computer program, in order to make it easy for others to use and modify.
- (d) Write a FORTRAN program which reads 30 rows of numerical data and provides a sum of all numbers in those data which are greater than 20.0 but less than 40.0. The program should also write the fraction of numbers, of the total set of numbers, that satisfy this criterion.
- (e) What factors contribute to the heat capacity of a metal?
- (f) Describe the Kirkendall experiment and how this proves that diffusion in the solid state occurs by a vacancy mechanism.
- (g) Why does the growth rate of a particle undergoing isothermal, one-dimensional, diffusion-controlled growth decrease as the particle gets larger?
- (h) Describe how hyperbolic tangents can be used to construct nonlinear models typical in neural network analysis. State one way in which overfitting to experimental data is avoided in neural network analysis.
- (i) Sketch a coarse scale representation of a diblock copolymer. What are the two main parameters of a mesoscale model of a melt of such a block copolymer. What type of structure is expected when a symmetric diblock copolymer melt phase separates? Write down the general expression of the mean squared end-to-end distance scaling for a polymer chain. How might the exponent of the phase separated diblock copolymer end-to-end distance relate to that of a homopolymer melt?
- (j) What are the potential benefits of a mathematical model of an industrial process? Give two examples to illustrate your answer.

SECTION B

2. Explain, in the context of binary solutions, what is meant by the term *chemical potential*. Hence justify the fact that the common tangent construction, on a free energy versus concentration plot, gives the equilibrium compositions of the phases.

Show how the diffusion coefficient can be written in terms of the chemical potential gradient rather than the concentration gradient. In what circumstances might the diffusion flux oppose the concentration gradient?

3. During the design of a mesoscale model of a polymer chain, the level of coarse graining is chosen such that the polymer is represented by a Gaussian chain. Explain in words the meaning of a *Gaussian chain* and of the orientational correlations of bonds along the chain.

Name two specific choices of mesoscale model you would consider for simulating solutions of such Gaussian chain polymers, and state three key features of each model. Give a general expression for the upper and lower bound of the time step which can be used in a Brownian Dynamics simulation of such a model, defining the terms. Given the fact that the relaxation time for bond rotations is 10^{-11} s, the segment length is $l = 1$ nm, and the diffusivity per segment is $D = 10^{-7}$ cm² s⁻¹, provide estimates for these upper and lower bounds.

4. Explain the concept of an *extended volume* in the context of the Avrami theory for overall transformation kinetics. Stating any assumptions, deduce the relationship between a change in the extended volume of the precipitate phase and the corresponding change in its real volume.

A phase α precipitates from γ in a reaction which involves nucleation at randomly located sites within γ . Assuming that the growth rate of the α is constant and isotropic, derive an expression which relates the volume fraction of α as a function of transformation time and the nucleation and growth rates.

5. Briefly outline the basis of the shear-lag model for load transfer in short-fibre composites. Use this approach to derive an expression for the critical fibre aspect ratio representing the shortest fibre length which can be fractured by imposing a large strain on the material.

In a short-fibre composite loaded parallel to the fibre axis, the contribution to the fracture energy from interfacial debonding is given by

$$G_{cd} = fsG_{cl}$$

where f is the fibre volume fraction, s is the fibre aspect ratio (length divided by diameter) and G_{cl} is the fracture energy of the fibre/matrix interface. Explain the limits within which this expression is valid.

SECTION C

6. (i) Describe how molecular solids are bonded. The Lennard–Jones potential is frequently used to model solid inert gases. Provide a justification for the functional form of each term in the potential. What is the range of validity of the potential and explain the principal computational advantages of its use.

The total energy per atom of a Lennard–Jones solid is given by

$$u(r) = 2\epsilon \left[\sum_i \left(\frac{\sigma}{p_{ij}r} \right)^{12} - \sum_j \left(\frac{\sigma}{p_{ij}r} \right)^6 \right]$$

where ϵ and σ are constants, $p_{ij}r$ is the distance between atoms i and j and r is the nearest neighbour separation.

Face-centred cubic (fcc) structure: $\sum_j p_{ij}^{-12} = 12.13$ and $\sum_j p_{ij}^{-6} = 14.45$

Body-centred cubic (bcc) structure: $\sum_j p_{ij}^{-12} = 9.11$ and $\sum_j p_{ij}^{-6} = 12.25$

Show that at equilibrium, the cohesive energy of the fcc structure is 4% lower than that of the bcc structure.

- (ii) Outline an *atomistic* method suitable for simulating the phase transition from a bcc to an fcc structure in the Lennard–Jones system as described in part (i). Your answer should identify the relevant thermodynamic state functions, give a brief summary of the simulation algorithm, contrast the method with another equivalent technique, and indicate how the simulation conditions differ from the calculation in part (i).

7. Explain what is meant by the terms *displacive* and *reconstructive* phase transformations, commenting particularly on the shape, chemical composition, and strains associated with each mechanism.

Describe the evolution of microstructure in the fusion zone of a steel weld as it cools from the austenite phase field, commenting specifically on the formation of allotriomorphic ferrite, Widmanstätten ferrite, acicular ferrite and martensite.

- (i) Which of these transformations is promoted by increasing the cooling rate?
- (ii) Derive an expression for the energy input per unit length (Q) during arc welding, in terms of the welding current, voltage, arc transfer efficiency and welding speed. How does the cooling rate depend on Q and on the original temperature T_0 of the substrate being welded?
- (iii) Why does the growth of allotriomorphic ferrite and Widmanstätten ferrite become sensitive to the carbon concentration as the concentration is reduced?