MASTER OF PHILOSOPHY   Modelling of Materials

Thursday 28 April 2005   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.*

Special and/or stationary 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) Explain the difference between a model and a theory in materials science, giving some examples of each, and discuss briefly how together they can form a synergy with experimental observation.

    (b) Describe briefly the ideas behind the Embedded Atom Method, including its physical origins, and state some of the advantages it has over other methods for simulating metallic systems.

    (c) Briefly outline the experimental methods for the determination of phase diagrams.

    (d) Show that if a material is in static equilibrium, $\sigma_{ij} = \sigma_{ji}$ $(i \neq j)$ for any stress state imposed on the material. A particular stress state imposed upon a material can be written in the form

    $$\sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} & 0 \\ \sigma_{12} & \sigma_{22} & 0 \\ 0 & 0 & \sigma_{33} \end{pmatrix}$$

    Find the three principal stresses of this stress state.

    (e) T^T, the transpose of the matrix T, is defined by

    $$\left(T^T\right)_{ij} = T_{ji}$$

    Write a FORTRAN 77 subroutine `tspose` which is called with a 10 × 10 real array representing the matrix as its argument. When the subroutine returns, the argument array should have been changed to the transpose of the original matrix.

    (f) Distinguish between the crystalline and amorphous states of matter. Give two examples of crystalline and amorphous solids. Describe a method that can be used to make amorphous solids.

(g) By considering diffusion driven by a free energy gradient rather than by a concentration gradient, show that in a binary *A-B* solution:

$$D_A = C_A M_A \frac{\partial \mu_A}{\partial C_A}$$

where for the solute A, D_A is the diffusion coefficient, C_A is the concentration, M_A is the mobility and μ_A represents the chemical potential. Under what circumstances is it necessary to consider the free energy gradient as the driving force for diffusion?

(h) Briefly discuss the construction of an artificial neural network in materials science. What are the advantages and disadvantages of using artificial neural networks compared to models based on physical laws?

(i) Summarise the advantages and disadvantages of numerical and analytical solutions for the thermal analysis of manufacturing processes.

(j) Explain how the *united atom approximation* can be used to accelerate the simulation of long chain alkane molecules using a classical molecular dynamics approach. Compare and contrast this method with other dynamical simulation techniques for predicting the structure of crystalline and amorphous polymers.

SECTION B

2. Describe the phenomenon of *Ostwald ripening* of precipitate particles
    in a matrix. What is the practical significance of the ripening?

    [15%]

    What is the driving force for the ripening? Use a sketch to illustrate
    the diffusional fluxes involved. Explain why some particles shrink,
    even as the overall dispersion coarsens. Sketch how the particle size
    distribution is expected to evolve with time.

    [25%]

    Precipitates of β phase (composed of B atoms) are dispersed in a
    matrix of α phase (composed of A atoms with some B in solid
    solution). The equilibrium concentration $X_\alpha(r)$ of B atoms in α at the
    interface with a spherical β particle of radius r is given by:

    $$X_\alpha(r) = X_\alpha(\infty)\left[1 + \frac{2\gamma V_m}{RT}\frac{1}{r}\right]$$

    where γ is the α-β interfacial energy, V_m is the molar volume, R is the
    molar gas constant and T is temperature. From this, making clear the
    assumptions in your derivation, show that the average precipitate
    radius $\bar{r}$ increases with time t according to

    $$\bar{r}^3(t) - \bar{r}^3(0) \propto t$$

    [30%]

    This analysis provides a basis for choosing a solute on which to base
    precipitation-hardening of a metal such that the rate of Ostwald
    ripening would be minimised. Which are the key parameters to
    consider?

    [15%]

    Discuss how the assumptions in the above derivation may be
    restrictive, and explain briefly how a full microstructural model could
    cope with greater complexity.

    [15%]

3.   The analytical solution for the Jominy end-quench test may be used to find the cooling rate dT/dt, at a fixed reference temperature, as a function of the distance x from the quenched end. The solution for the cooling rate is:

$$\frac{dT}{dt} = -\frac{C}{x^2}$$

where C is a dimensional constant, which depends on the selected reference temperature.

A finite element (FE) analysis was conducted with the same boundary conditions as for the analytical solution, but with a domain equal to the actual length of the sample, 120 mm. Selected results from the FE analysis for the magnitude of the cooling rate at the same reference temperature are given in the table below.

Distance from quenched end, x (mm)	Cooling rate (K/s)
2	631
5	100
10	25.1
20	6.31
40	2.24
80	1.26
120	1.0

   (a)   State the boundary conditions for both analytical and FE analyses, and suggest a suitable number and type of element for the FE analysis.

[20%]

(TURN OVER

(b)   Plot the FE results for cooling rate against distance from the quenched end on log-log scales, and compare the FE data with the behaviour predicted by the analytical solution. Explain the discrepancy between the two.

[50%]

(c)   Use your plot to find the value of the constant C, by fitting the analytical result to the FE solution where appropriate.

[30%]

4.   Compare and contrast the linear regression method with general neural network analysis. Your answer should include a full description of both techniques and some examples of their application.

[100%]

5.   Write down an expression for the Lagrangian, L, of a collection of N particles, expressed as the difference of their kinetic and potential energies. Show that Newton's second law of motion follows from substituting L into the Euler-Lagrange equation:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}_i} - \frac{\partial L}{\partial x_i} = 0$$

[30%]

If L is augmented by an extra co-ordinate ς, which evolves in time so as to minimise the difference between the instantaneous kinetic and statistical temperatures, T_K and T_S respectively, then the modified equations of motion become:

$$\dot{\underline{r}}_i = \underline{p}_i / m_i$$
$$\dot{\underline{p}}_i = \underline{F}_i - \varsigma \underline{p}_i$$
$$\dot{\varsigma} = \frac{1}{\tau_T^2}\left\{T_K(t)/T_S - 1\right\}$$

Define carefully each of the terms in the above equations, and explain the significance of the parameter τ_T. Describe in practical terms how to choose τ_T in order to obtain the most efficient sampling of states from a constant temperature molecular dynamics simulation. What is the conserved quantity of the resulting ensemble?

[50%]

What advantages and disadvantages does the deterministic scheme above have over stochastic methods for regulating temperature in molecular dynamics simulations?

[20%]

SECTION C

6. Layers of solute-rich β phase are found to thicken as a function of time during isothermal transformation from α. Using the data given in the table below, assess what the rate-controlling process is for the motion of the β/α interface.

Thickness of β layer / μm	Time / s
0	0
0.47	2
0.64	4
0.90	8
1.28	16

[20%]

Illustrate the distribution of solute ahead of the transformation interface, marking on your diagrams the equilibrium compositions of the parent and product phases ($C^{\alpha\beta}$ and $C^{\beta\alpha}$ respectively) and the average composition C_0.

[20%]

One of the conditions for the diffusion-controlled growth of β is that

$$\left(C^{\beta\alpha} - C^{\alpha\beta}\right)\frac{\partial x^*}{\partial t} = D\frac{\partial C}{\partial x}\bigg|_{x=x^*}$$

where D is the diffusivity of the solute in the matrix, t is time and x is a co-ordinate normal to the interface. x^* represents the position of the interface, where the concentration gradient is evaluated.

Explain the origin of the equation and derive the relationship between x^* and t. Identify any approximations or assumptions that you make.

[60%]

7. 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 solutions? Illustrate how this justifies the common tangent construction which is used to find the equilibrium compositions of phases in contact.

[50%]

A binary solid-solution contains a random dispersion of n B-atoms and $N - n$ A-atoms. When N is set to equal Avogadro's number, the molar configurational entropy of mixing is given by:

$$\Delta S_M = -kN\left[(1 - x)\ln\{1 - x\} + x\ln\{x\}\right]$$

$$= -kN\left[\left(\frac{N - n}{N}\right)\ln\left\{\frac{N - n}{N}\right\} + \frac{n}{N}\ln\left\{\frac{n}{N}\right\}\right]$$

where k is the Boltzmann constant and x is the mole fraction of B atoms. During a nucleation event, a cluster of t B-atoms forms. Show that the change in configurational entropy when a single such cluster forms in this otherwise random solution is

$$\Delta S \cong k(t - 1)\ln\{x\}$$

[40%]

END OF PAPER