

MODELLING OF MATERIALS (1)

*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) Describe the differences between the values which can be stored in FORTRAN integer and real variables. Write a FORTRAN program to print out the sum of the reciprocals of the integers from 1 to 100, inclusive.
- (b) It is recommended during K_{Ic} fracture toughness testing, that the minimum sample thickness, B , necessary to achieve plane strain fracture is given by $B > 2.5(K_{Ic}/\sigma_y)^2$, where σ_y is the yield strength. Discuss this condition in terms of the size of the plastic zone at the crack tip. What other dimensions are controlled and why?
- (c) The elastic modulus is an intrinsic property of a material whereas the ability of the material to resist plastic deformation is an extrinsic property. Explain what this statement means and describe the techniques appropriate for modelling each of these properties.
- (d) Dendritic microstructures are commonly formed during the casting of alloys. Why is this?
- (e) Describe the difference between an *ideal* solution and a *regular* solution. Why is the configurational entropy term in the regular solution model to be regarded as approximate?
- (f) State the principal steps involved in the development of a computer model to deal with a problem or phenomenon in materials science.
- (g) What are the principal terms comprising the total energy of a solid when described using density functional theory? In order to obtain equilibrium configurations the total energy must be minimised. What is the traditional approach to minimising the total energy and which method is used in modern calculations?
- (h) Under what circumstances is the standard entropy change for a given reaction independent of temperature?
- (i) In the context of molecular simulations, define and explain the difference between statistical temperature and kinetic temperature.
- (j) Explain the advantages and disadvantages of modelling the structure of materials at the atomistic level, giving two examples to illustrate your answer.

SECTION B

2. Distinguish between the terms *strength* and *toughness*. Describe ways of measuring both of these quantities for metallic alloys.

The stress intensity K_1 in mode 1 loading in an infinite plate containing a centre-crack of length $2a$ is given by

$$K_1 = \sigma_{app}(\pi a)^{\frac{1}{2}}$$

where σ_{app} is the applied stress. The corresponding relationship for a semi-infinite plate containing an edge crack of length a is

$$K_1 = 1.12\sigma_{app}(\pi a)^{\frac{1}{2}}$$

Comment on why it is necessary to include a factor 1.12 in the second equation.

A very large plate of a high strength aluminium alloy contains an edge crack of length 40 mm. Given that it fails at an applied stress of 100 MPa, calculate the fracture toughness of the alloy.

How would this calculation be modified if the edge crack occurred at a large circular hole machined in the plate?

3. Describe the nature of the bonding in ionic crystals. Using suitable sketches, show how the electrons in an ionic crystal such as KCl are spatially distributed and also how they occupy the allowed energy levels in the band structure of the material. How can the spatial distribution of the electrons be used to formulate interatomic potentials for atomistic modelling?

Let the total energy per ion pair in a binary ionic crystal be given by

$$u(r) = -\frac{\alpha q^2}{r} + Cr^m$$

where r is the nearest neighbour separation, q is the ionic charge and α , C and m are constants.

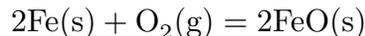
- (i) Derive an expression for C in terms of the equilibrium separation r_0 .
- (ii) Show that the cohesive energy per ion pair at equilibrium is given by

$$u(r_0) = -\frac{\alpha q^2}{r_0} \left(\frac{m+1}{m} \right).$$

- (iii) If 90% of the cohesive energy of KCl is Coulombic, determine an appropriate value for m .

4. Explain why the free energy of formation of metallic oxides is less negative at high temperatures than that at room temperature and yet metals oxidise more rapidly at high temperatures.

The standard free energy change for the following oxidation reaction:



is given by:

$$\Delta G^0(\text{J mole}^{-1} \text{ of oxygen}) = -265000 + 70T$$

where T is the absolute temperature.

Calculate the equilibrium constant K for the above reaction at 1000 K. What is the equilibrium partial pressure of oxygen when pure Fe is in contact with pure FeO at the same temperature. If Fe is made impure, will the equilibrium partial pressure of oxygen increase, decrease or remain the same?

5. What is meant by the term *force field* in the context of molecular simulations? Write down a suitable force field expression for modelling the dynamics of a long-chain polymer molecule, carefully defining all the terms used.

Explain the principles of the rotational isomeric state (RIS) model for generating realistic chain configurations, including an analytical expression that defines the RIS temperature.

SECTION C

6. Describe two processes which might control the rate at which an interface migrates during the isothermal growth of a precipitate (β) whose chemical composition is different from that of the parent phase (α). In each case, 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 .

One of the equations applying during the diffusion-controlled growth of a solute-rich precipitate β is as follows:

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

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

Explain separately the meanings of the left and right sides of this equation, and hence the origin of the equation.

Assuming that the concentration gradient in the matrix is constant, derive an equation relating x^* (in effect the thickness of the precipitate) to time, D , $C^{\alpha\beta}$, $C^{\beta\alpha}$ and C_0 (the composition of the matrix prior to precipitation).

Is it reasonable to suppose that the growth rate $\partial x / \partial t$ tends to infinity as $C^{\beta\alpha} \rightarrow C_0$?

In what circumstances would this equation fail?

7. Describe the purpose of the Jominy end-quench test for steels.

A finite element model of the Jominy end-quench test is constructed as shown in Fig. 1. The model uses two one-dimensional linear elements of equal length, with constant thermal properties. The bar is initially at a uniform temperature of 850°C and is quenched on one end with water at a temperature of 20°C . Perfect heat transfer is assumed at the quenched end and perfect insulation on the remaining faces. The calculated nodal temperatures for times after quenching of 10, 100 and 1000 s are tabulated below.

	Node 1	Node 2	Node 3
10 s	20.0°C	808.4°C	847.6°C
100 s	20.0°C	559.8°C	726.2°C
1000 s	20.0°C	51.9°C	65.1°C

- (i) State the material properties which must be specified to conduct the finite element analysis and explain how the boundary conditions would be specified.
- (ii) Plot the temperature predicted by the finite element model against distance from the quenched end, and explain the main limitations of this model. How could the analysis be refined?
- (iii) Explain which (if any) of the various solutions might be appropriate for: (a) estimating the number of tests which could be conducted in one day; (b) predicting the cooling rate to an accuracy of 1°C s^{-1} at a position 1 mm from the quenched end, on the outer surface of the bar; (c) deciding if the test could be adapted to investigating cooling rate effects in heat-treatable aluminium alloys.

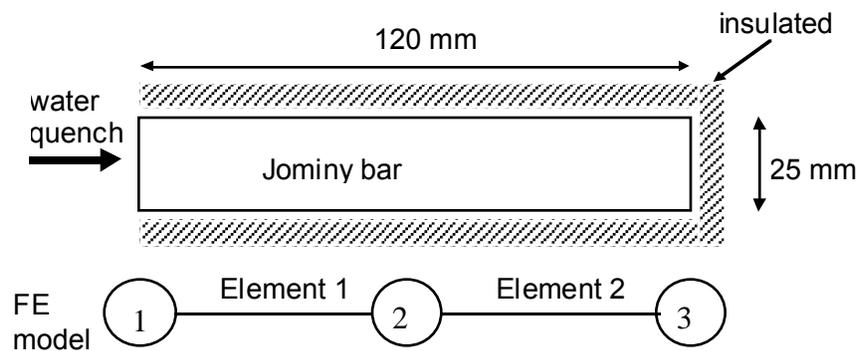


Fig. 1