MASTER OF PHILOSOPHY   Modelling of Materials

Wednesday 26 April 2006   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 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) Define the following terms: *Bravais lattice*, *motif* and *conventional unit cell*. Draw a projection onto (100) of the conventional unit cell for the cubic diamond structure. What is the rotational symmetry about a [100] axis passing through a carbon atom?

   (b) Discuss briefly the physical basis of the Embedded Atom Method used to model metals and indicate the general form of the embedding function.

   (c) Discuss briefly the principal differences between a deterministic and stochastic computer model in materials science.

   (d) "Eco awareness" is increasingly necessary for builders and manufacturers. What is *eco selection* and how can it be modelled? Illustrate your answer by considering eco selection for:
   (i) family cars;
   (ii) wooden chairs;
   (iii) multi-storey car parks.

   (e) The determinant, $|A|$, of a 2×2 matrix is given by:

$$|A| = \sum_{i=1}^{2}\sum_{j=1}^{2} \varepsilon_{ij} A_{1i} A_{2j} \qquad (*)$$

   where $\varepsilon_{12} = 1$, $\varepsilon_{21} = -1$, and $\varepsilon_{11} = \varepsilon_{22} = 0$.

   Write a FORTRAN function which, when passed a 2×2 real array representing a matrix, uses the formula (*) to evaluate the determinant of the matrix and returns it as a real value.

   Would you use the formula (*) above in practice to evaluate the determinant of a 2×2 matrix?

(f) Explain what is meant by *quantum mechanical tunnelling*. Briefly describe two cases in which it is manifest.

(g) Discuss the role of *thermal importance sampling* in the Metropolis Monte Carlo algorithm for atomistic simulations.

(h) Distinguish between *diffusive* and *hydrodynamic* behaviour in mesoscale simulations, and describe a material system in which this difference gives rise to observable consequences.

(i) Explain how the use of a Schottky metal gate on the surface of a GaAs-based two-dimensional electron gas can be used to demonstrate the quantisation of the ballistic resistance.

(j) A block of isotropic elastic material is constrained so that the principal strains ε_2 and ε_3 are both zero. It is then loaded in uniaxial compression with a principal stress σ_1. Determine the 'effective modulus', σ_1/ε_1, of the material in terms of the Young's modulus, E and Poisson ratio, ν. Comment briefly on the significance of this result for a material whose Poisson's ratio is ≈ 0.5.

SECTION B

2. Artificial neural networks can be applied to fit model functions to data in circumstances where simpler methods such as polynomial regression could also be used. Using an example, discuss the strengths and weaknesses of each method, including practical considerations. Indicate clearly the difficulties associated with neural network modelling and how they can be overcome. Give some recommendations as to which method might be used depending on the details of the problem.

[70%]

The following summarises the content of a paper which was rejected from publication: "The strength of non-woven fabrics was modelled using a neural network with three hidden units, using the five most relevant inputs variables (as identified in a first phase of work). A total of fifteen data points were collected and used to train the model. Comparisons between the predictions and the data points show good agreement." Do you think the referee was justified in rejecting the paper? Explain your reasoning as fully as possible.

[30%]

3. A finite element analysis has been conducted to model the Jominy end-quench test. The sample was a 25mm diameter steel bar of length 120mm. Details of the analysis were as follows:

(i) two linear elements of equal length;
(ii) constant thermal properties;
(iii) initial uniform temperature of 850ºC;
(iv) perfect quench at one end to 20ºC;
(v) perfect insulation over the remaining surfaces.

(a) Briefly summarise the purpose of the Jominy end-quench test.
[15%]

(b) After 100 seconds, the predicted temperatures at the nodes at x = 60 and 120mm (measured from the quenched end) are 560 and 726ºC, respectively. Sketch the temperature profile $T(x)$ predicted by the analysis.
[25%]

(c) The analysis is repeated several times, making one change from the initial case (b) above. The changes are not retained each time, so that the effect of varying single aspects of the analysis can be explored. For each of the following changes to the initial analysis, sketch the original and the new temperature profiles (on a new figure each time):

(i) time after quench = 1 second;
(ii) four linear elements of equal length;
(iii) two quadratic elements of equal length;
(iv) boundary condition at the quenched end: heat transfer coefficient for moderately good heat transfer.
[40%]

(d) Summarise in what respects the analytical solution for the Jominy end-quench test differs from the initial FE analysis. Illustrate your answer by sketching the expected temperature profile after 100 seconds, as in part (b).
[20%]

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4. The deformation tensor e_{ij} associated with slip on a single slip system is given by:

$$e_{ij} = \gamma n_j \beta_i$$

where γ is the shear angle (assumed to be small), $\mathbf{n}$ is a unit vector normal to the slip plane and $\boldsymbol{\beta}$ is a unit vector in the slip direction. The components of $\mathbf{n}$ and $\boldsymbol{\beta}$ are defined in a reference set of orthonormal axes.

Explaining your reasoning, write down the components of the strain tensor ε_{ij} associated with the deformation. What is the magnitude of the trace of the strain tensor?

[30%]

Lithium fluoride, LiF, has a cubic F crystal structure. At room temperature, the slip systems are $\{110\}\langle 1\bar{1}0\rangle$. Write down the strain tensors corresponding to slip on the physically distinct slip systems. How many of these slip systems are independent? What can you deduce about the ductility of LiF?

[70%]

5. A isolated atom exists in one of three states, denoted by quantum number $n = 0, 1, 2$: the ground state ($n = 0$), and two excited states with energies ε ($n = 1$) and 2ε ($n = 2$) relative to the ground state. The degeneracy of each state is given by $2n + 1$.

Explaining your reasoning, compute the average internal energy $<U>$ of the isolated atom in thermal equilibrium at temperature $T = \varepsilon / k_B$, where k_B is Boltzmann's constant.

[30%]

Derive an expression for the high temperature functional form of the isovolumetric heat capacity of the system.

[50%]

Describe a method for calculating the above quantities for a system of N atoms interacting via some potential energy function (note that you are not expected to perform any explicit calculations).

[20%]

SECTION C

6. Describe, with the aid of sketches, the four main steps in the fabrication of a single electron transistor (SET) made using highly doped silicon-on-insulator (SOI).

[20%]

(a) Describe what is meant by *Coulomb blockade* in a small island capacitor. Sketch the current-voltage characteristics of the Coulomb blockade.

[20%]

(b) Discuss the influence of the following on the observation of Coulomb blockade effects:

(i) the charging energy of the island,

(ii) the resistances of the tunnel barriers.

[20%]

(c) Estimate the maximum temperature for which Coulomb blockade will be observed in a SOI-based SET with an island diameter of 60 nm. You may neglect any other contributions to the island capacitance and confinement effects.

[40%]

[The self capacitance C of a circular disc of silicon, embedded in SiO_2, is given by $C = 8\varepsilon_r\varepsilon_0 r$, where r is the radius of the disc, $\varepsilon_r = 3.9$ is the relative permittivity of SiO_2, $\varepsilon_0 = 8.8\times10^{-12}$ F m^{-1} is the permittivity of free space, and Boltzmann's constant $k_B = 1.38\times10^{-23}$ J K^{-1}. The charge on an electron is 1.6×10^{-19} C].

7. Discuss the classes of materials for which the pair potential approximation used to perform atomistic simulations is justified and those for which it is not. Include sketches of the electron density distributions in the materials to support your arguments.

[10%]

Consider the following pair potential employed in an atomistic simulation:

$$U(r) = -Ar^{-n} + Br^{-m}$$

where *A, B, n* and *m* are positive constants.

(a) Indicate the physical significance of the two terms in *U(r)*.

[10%]

(b) The elastic modulus of a simple cubic crystal extended along one of its cell edges is given by:

$$E = \frac{1}{r_0}\frac{d^2U}{dr^2}\bigg|_{r_0}$$

where r_0 is the equilibrium inter-atomic spacing. Determine an expression for *E* using the pair potential, and show that the condition for crystal stability is that $m > n$.

[30%]

(c) Show that the ratio of the spacing r_f at the maximum attractive force to the equilibrium spacing r_0 is given by:

$$\frac{r_f}{r_0} = \left(\frac{n+1}{m+1}\right)^{\frac{1}{n-m}}$$

Sketch the form of the force-distance curve for the potential and label the spacings r_f and r_0. Use the sketch to indicate the elastic modulus *E* for a weakly bonded crystal and a strongly bonded crystal.

[40%]

(d) Consider the two potentials for which $(n, m) = (6, 12)$ and $(n, m) = (1, 12)$. By determining ratio r_f / r_0, find the maximum tensile strain before bonds break in both cases. Comment on the values you obtain in relation to the different classes of crystal the two potentials represent and also experimental observations. [10%]

END OF PAPER