Master of Philosophy

MODELLING OF MATERIALS

Lecture 1 (ALG)
Introduction to materials. States of matter. Equilibria. Effect of temperature and pressure.

Lectures 2, 3 (HDB)
Introduction to crystallography, the lattice, the Bravais lattices, directions, planes, the reciprocal lattice, electrons in metals, symmetry, symmetry operations, crystal structure, interstices, defects.

Lectures 4, 5 (REC)
Introduction to stress and strain.

Lecture 6 (PJH)
Definition of materials modelling and connections to theory and experiment. The objectives of materials modelling (materials prediction, process optimisation, materials design). Model selection – general considerations.

Lecture 7 (PJH)

The importance of spatial and temporal length scales in materials modelling (characteristic materials processes and corresponding scales).The hierarchy of materials models based on length scale (connections to problems in physics, chemistry and engineering). Bridging the length scales. The central role of algebraic, differential and integral equations in materials modelling on different length scales (review of typical equations, modelling methods and applications).

Lecture 8 (PJH)
The development and construction of a physical model for a material (a review of the important stages including choice of length scale, model approach, model parameters, model interrogation and model validation). A summary of technical issues that need to be considered (boundary conditions, error tolerance, data analysis and visualisation).

Lecture 9 (MRM)
Introduction to computing in the department. Passwords and general administration. Windows NT, IRIX and Linux: logging in, file access, printing. UNIX. File system structure; directories; file and directory commands. Editing; compiling; simple use of make. Redirecting input and output.

Lecture 10-12 (MRM)
FORTRAN. Integer, real and double-precision values, variables, arithmetic assignment, loops, conditions, data statements.

Arrays, subroutines and functions, arguments, common blocks.
DATA and FORMAT statements. Use of pgplot graphics library.

COMPUTING EXERCISES

2. Introduction to basic computing on departmental PC's and SGI workstations. File and directory structure, file manipulation, file editing, file processing and execution. Example of running a simple Fortran program and displaying the results (cooling curves). Illustration of the numerical solution of a first order differential equation by the Euler method. (MRM)

(10) Writing and modifying a simple Fortran code to illustrate the analytical solution to a first order differential equation (cooling curves). Comparison with the numerical solution and discussion of accuracy. Re-programming to take into account solidification and the latent heat of fusion. (MRM).

READING MATERIAL

13 *The Cambridge Guide to the Material World*, R. Cotterill, CUP, 1985
14 *Computational Materials Science*, D. Raabe, Wiley-VCH, 1998 (Chaps 1 & 2 only).

Lecture 1 (PJH)
Microscopic systems and interaction potentials. The quantum mechanical and classical Hamiltonians. The many-body expansion of the effective classical interatomic potential. Decomposition into pair, triplet and higher order terms.

Lecture 2 (PJH)
Classification of solids. Molecular, ionic, covalent and metallic bonding. Simple band structure picture. The spatial distribution of valence electrons. The nature of interaction potentials in different solids.

Lecture 3 (PJH)
Effective pair potentials for molecular solids. The van der Waals interaction. The Lennard-Jones potential for inert gas crystals. The equilibrium density, cohesive energy and bulk modulus of Lennard-Jonesium. Examples of Lennard-Jones simulations.

Lecture 4 (PJH)
Effective pair potentials for ionic solids. The electrostatic energy and the Madelung constant. Atomic polarizability and the shell model.

Lecture 5 (PJH)
Effective three-body potentials for covalent solids. The van der Waals triplet interaction. Keating's valence force field. Stillinger - Weber's parameterised three-body potential for silicon.

Lecture 6 (PJH)
Effective many body potentials for metals. Density dependent potentials. Effective medium theory. The glue model. The embedded atom model.

Lecture 7 (PJH)
Review of free electron theory: wave equation, wave vectors and k-space, energy levels, Fermi energy, density of sates, Fermi-Dirac distribution function. Successes and failures of free electron theory.

Lecture 8 (PJH)
Electrons in crystals: Bloch's theorem, energy bands and gaps, intepretation in terms of Bragg's law. The electron energy dispersion E(k) in one dimension.

Lecture 9 (PJH)
Zone scheme representations of E(k). Brillouin zones in two and three dimensions. The number of allowed states in a band and the distinctionbetween metals and insulators. Band overlap.

Lecture 10 (CJP)
Kohn-Sham equations, periodic boundary conditions, super-cells, plane waves and pseudopotentials.

Lecture 11 (CJP)
Minimisation approaches, forces, stress, geometry optimisations and molecular dynamics.

Lecture 12 (CJP)

Non-structural properties: phonons, spectroscopies. Applications: theoretical strength and cleavage of diamond.

Lecture 13 (CJP)
Applications: core level / optical spectroscopies. Prediction of carbon polymorphs. How hard is CNx?

COMPUTING EXERCISE

Use of the CASTEP module within CERIUS2 to simulate the bulk properties of silicon from first principles.

READING MATERIAL

Introduction to Solid State Physics, C. Kittel (Wiley 1986) Chaps 3, 6,7,8,9
Solid State Physics, NW Ashcroft and ND Mermin (Saunders College 1976) Chaps 19, 20
Interfaces in Crystalline Materials, AP Sutton and RW Balluffi (OUP 1995) Chap. 3

[12 lectures – JAE]

Lecture 1

Introduction to materials modelling at the molecular scale. Brief review of equilibrium thermodynamics: state functions, Maxwell relations and laws of thermodynamics. Thermodynamic definition of temperature, principle of equipartition, diffusive equilibrium and the grand potential.

Lecture 2

Review of classical statistical mechanics for systems in equilibrium, including the Gibbs definition of entropy, the MaxEnt principle and a derivation of the Boltzmann distribution. Concept of the partition function, fluctuation-disspation theorems and derivation of the ideal gas equation from its partition function.

Lecture 3

Reminder of the partition function, and application to a diatomic gas. Discussion of non-separable partition functions, and the role of computer simulation. Use of reduced units in simulations to avoid duplication of equivalent thermodynamic states.

Lecture 4

Monte Carlo methods I. Brief history of MC methods. Summary of basic MC algorithm. MC as a Markov process. The Metropolis acceptance scheme. Metropolis MC in the canonical ensemble. Examples of how to apply MC, including Buffon's needle and the 2D Ising model. Techniques for accelerating equilibration in large or complex systems: cluster moves, particle exchange.

Lecture 5

Monte Carlo method II. Advanced MC applications, including microcanical and grand canonical simulations, configurationally-biased sampling techniques and kinetic MC. Thermodynamic integration to calculate free energies.

Lecture 6

Force calculations and force fields for atomic and molecular systems. Methods for force field parameterisation, using experimental data and ab initio or semi-empirical quantum mechanical calculations.

Lecture 7

Molecular dynamics methods I. Summary of basic MD algorithm for continuous and impulsive systems. Discussion of criteria for good integrators: time reversibility, symplecticity and energy conservation. Verlet and predictor-corrector methods as examples. Some tricks of the trade used to carry out efficient MD simulations.

COMPUTING CLASS 1

Lecture 8

Molecular dynamics method II. Canonical MD using extended an Lagrangian. Isothermal-isobaric and isothermal-isenthalpic MD. Fast MD of macromolecules using united atoms approximation, constraint dynamics and rigid bodies. Multiple time step algorithms.

Lecture 9

Case study: Monte Carlo lattice modelling of polymers. Introduction to the lattice chain model and polymer chain statistics. Validation of lattice chain MC simulations using random walk statistics and reptation theory. Applications of the lattice chain model.

COMPUTING CLASS 2

Lecture 10

Visualising and and quantitative analysis of molecular simulations. Structural properties: radial distribution functions, velocity autocorrelation functions, orientational order parameters. Dynamic properties: mean-squared displacement, diffusion coefficients. Simulated X-ray scattering and IR spectra. Connolly surfaces and free volume.

Lecture 11

Case study: Molecular dynamics model of solvent diffusion in polymers. The glass transition, and how to simulate it using MD. Scaling laws and time-temperature superposition. Motion of penetrants in a glassy polymer, and the Vogel-Fulcher law. Effective temperature and non-equilibrium simulations.

COMPUTING CLASS 3

Lecture 12

Methods for simulating systems out of equilibrium. Non-equilibrium molecular dynamics simulations. Non-equilibrium diffusion coefficients and shear fields using linear response theory. Lees-Edwards boundary conditions. Hybrid MC/MD methods, including Anderson thermostat and grand canonical MC/MD.

COMPUTING EXERCISES

1. Modelling of phase separation in a binary Lennard-Jones fluid. (JAE/KLA/AIA – 9/11/2001 09:00-11:00)

2. Monte Carlo lattice model of polymer welding. (JAE/KLA/AIA – 16/11/2001 09:00-11:00)

3. Molecular dynamics of solvent diffusion through a glassy polymer. (JAE/KLA/AIA – 23/11/2001 09:00-11:00)

<u>Software resources required</u>

Cerius^2 4.2 Visualiser, BUILDERS, OFF SETUP, OFF METHODS and POLYMER 1 modules (MSI)
Lattice model code (Polymer Group)

Lecture 1 (HDB)
The thermodynamic functions: internal energy, enthalpy, entropy, heat capacity, Helmholtz and Gibbs free energies. Allotropic phase transformations. (HDB).

Lecture 2 (HDB)
Two-component systems, the chemical potential, activity, phase transformations in alloys, common tangent construction, driving force diagrams and their interpretation. (HDB).

Lecture 3 (HDB)
Solution theory: mechanical mixtures, ideal solutions, regular solutions, order-disorder transformations.

Lecture 4 (HDB)
Case study of mechanical alloying.

Lecture 5 (HDB)
Computer calculations of phase diagrams, stoichiometric phases, interstitial solutions, generalised regular solution models, magnetic effects, Zener ordering.

Lecture 6 (HDB)
Thermodynamics of irreversible processes, reversibility, the linear laws, multiple irreversible processes, Onsager reciprocal relations, limitations, modelling of diffusion (HDB).

Lecture 7 (HDB)
Quasichemical solution models.

Lecture 8 (DJF)
Determination of phase diagrams. Cooling curves for single component systems. Cooling curves for two component systems. Inverse rate curves. Dilatometry. Electrical conductivity. Examples of phase diagrams. Thermodynamics of phase diagrams. Free energy curves. Phase rule. Relationship between free energy curves and phase diagrams.

Lecture 9 (DJF)
Prediction of phase diagrams. Ideal and regular solution models. Effect of different values of Ω on phase diagrams. Prediction of metastable phases.

EXAMPLES CLASS

Use and abuse of MTDATA (HDB)

RECOMMENDED BOOKS:

1. *Chemical Metallurgy* - J.J Moore (Butterworth)
2. *Introduction to Materials Thermodynamics* - DR Gaskell (McGraw-Hill)

Lecture 1 (JAE)
Length scales of modelling and meaning of mesoscale and multiscale, the role of noise: recap of fluctuation-dissipation theorem and Langevin equation, distribution functions. Two concepts: (a) mesoscale as coarse-grained molecular scale, (b) mesoscale as continuum with microstructural complexity. Basic hydrodynamics.

Lecture 2 (JAE)
Removing atomic degrees of freedom by grouping atoms in units, Example of polymers: United atoms, Gaussian chain, Bead-spring chain, Dumbbell model. Simple scaling relationships. Parameterisation of length scales and interactions.

Lecture 3 (JAE)
Lattice methods: Lattice chain simulations, Ising model, Monte Carlo modelling of directors, Cellular automata, Lattice Boltzmann technique. Hydrodynamics in mesoscale methods. Examples.

Lecture 4 (JAE)
Off-lattice methods: Brownian dynamics simulations, Dissiplative Particles Dynamics simulation. Examples.

Lecture 5 (JAE)
Density functional approaches, dynamic density functional method, and MesoDyn software. Examples.

Lecture 6 (JAE)
Why multiscale modeling. Examples of structural hierarchies. Examples of multiscale modeling: Prediction of nanostructures in block-copolymers (molecular modelling for interaction energies and chain stiffness + mesoscale modeling of structures) Hierarchical modeling of liquid crystal polymer materials (molecular torsion potentials + microstructural modeling of directors), Multiscale modelling of fracture and crack propagation (FEM combined with MD)

Lecture 7 (HDB)
Multiscale modelling in the design of creep-resistant steels.

DEMONSTRATION:

13 Determine the mesoscale structure of a polymer blend (use DPD or MesoDyn).
14 Effect of adding another ingredient, e.g. adding a compatibilizing block copolymer.

COURSE MP6: KINETICS AND MICROSTRUCTURE MODELLING

Lecture 1 (ALG)
Introduction to microstructure, making links with Course 1 (General Methodology), Course 4 (Thermodynamics and Phase Diagrams), and Course 5 (Mesoscale and Multiscale Modelling). The elements of microstructure — grains, domains, twins, precipitates and phase constitution, dislocations, composition variations. Comparison with artificial composites. The importance of microstructure (some examples) — grain-size strengthening, precipitation hardening, tempering of martensite, Cu-Nb-Sn superconducting wires, metallic multilayers for giant magnetoresistance.

Lecture 2 (ALG)
Exploitation of phase transformations for the development of microstructure, making links with processing (later Courses 7 and 8). The importance of and limitations of thermodynamics. The elements of kinetics — atomic diffusion, motion of interfaces, nucleation and growth. Relevance for development of, and stability of, desired microstructure. Atomic diffusion mechanisms — interstitial, substitutional. Main characteristics of diffusion — the random walk, distance □ $\sqrt{\text{time}}$, thermal activation, Arrhenius law.

Lecture 3 (HDB)
Fick's first and second laws, the diffusion equation. Solving the diffusion equation — thin-film solution, semi-infinite solids. Interstitial, substitutional and vacancy diffusion. Activation energies and vacancy concentrations. Diffusion and microstructure — fast diffusion paths, grain-boundary, free-surface and lattice diffusion.

Lecture 4 (HDB)
Thermodynamics of diffusion, chemical potential and atomic mobility, ideal and non-ideal solutions, concepts of zero diffusivity, negative diffusivity and uphill diffusion, spinodal decomposition. Numerical solutions of the diffusion equation. Finite-difference methods. Examples of applications.

Lecture 5 (HDB)
Diffusion and moving-boundary problems. Local equilibrium, mass conservation conditions, Zener approximation and one-dimensional diffusion-controlled growth, parabolic growth, the effect of soft-impingement, effect of concentration dependence of diffusivity, capillarity effects, growth of cylinders, needles, plates.

Lecture 6 (ALG)
Nucleation. Examples of the importance of nucleation — inoculation of castings, microstructure in steels, nucleation of domains. The classical theory, homogeneous and heterogeneous nucleation. The steady state nucleation frequency — Volmer-Weber and Becker-Döring analyses. Transient effects in nucleation. Problems of modelling nucleation — lack of data on key parameters.

Lecture 7 (HDB)
Growth. Examples of the importance of growth rates and growth morphologies — spheroidal graphite in cast irons, organized versus chaotic microstructures. Growth in solidification — diffusion-limited and collision-limited, faceted or non-faceted, survey of rate-controlling factors.

Growth in the solid state — displacive and reconstructive transformations. Rate limiting steps for growth, stress and strain effects.

Lectures 8,9 (HDB)
Overall transformation kinetics. Homogeneous and heterogeneous reactions. The concept of extended volume. Johnson-Mehl-Avrami kinetics. Survey of different examples. Limitations of the JMA approach. Modelling of simultaneous transformations.

Lecture 10 (HDB)
Non-isothermal kinetics, modelling of calorimetry data. Isothermal transformation (TTT) diagrams. Isokinetic reactions. Continuous cooling (CCT) diagrams.

Lecture 11 (ALG)
Processes where size dispersion is important. Grain growth — analysis of kinetics in 2D and 3D, normal and abnormal growth, stagnation, applications of grain growth modelling in microelectronics and other fields.

Lecture 12 (ALG)
Ostwald ripening — significance, mathematical analysis, rate-controlling factors, importance of modelling.

Lecture 13 (ALG)
Introduction to the importance of grain structure and its control. A case study on grain refinement in metal castings by addition of inoculants. Length scales for diffusion of heat and solute, the assumption of an isothermal melt. Undercoolings for nucleation and for free growth, rate control by free growth. Example of refining of aluminium, showing how modelling can give quantitative predictions for grain size as a function of key processing parameters. Limitations of such modelling.

Lecture 14 (HDB)
Case study on solid-state transformations in creep-resistant steels, mechanisms of carbide and intermetallic compound formation, simultaneous transformations, combined precipitation and coarsening reactions.

Lecture 15 (HDB)
Introduction to phase-field modelling. Phase-field parameters and the definition of an interface. Free energy functional and derivation of the equilibrium state. Examples: solidification, welding, solid-state transformations

EXAMPLES CLASS

At the end of the course, this will be used to go through two Question Sheets with the students.

COMPUTING EXERCISES

1. JMA simulation, CCT diagrams (HDB)

3. Thermal modelling of grain-refinement in solidification (ALG)

6 lectures (HRS, HKDB, ST)

Lecture 1 (HRS)
Modelling problems in materials processing. Fundamental ideas (illustrated through heat flow): governing differential equations, boundary conditions, FE approximation. Analytical or numerical methods? Finite element discretisation. Introduction to computing class: heat flow analysis of Jominy end-quench. Concept of appropriate simplification of the problem.

Lectures 2(+3) (HKDB)
Thermal FE analysis. 1D elements and thermal stiffness matrix. Hand calculation of steady-state 1D problem: conduction through cavity wall. Steady-state versus transient problems. Mechanical FE analysis. 1D elements in 1D and 2D problems (pin-jointed frame). Stiffness matrix. Generalisation to 2D, 3D elements and from force/displacement of pin-jointed members to stress/strain of continuum. Shape functions.

Lecture 4 (ST)
Implementation issues: choice of element type, mesh generation and re-meshing, hour-glassing, coupled or decoupled thermal/mechanical analyses…..

Lecture 5 (HRS)
Industrial process modelling: the role of FE analysis. Integrated FEA and microstructural modelling. Case study 1: Direct-chill casting of aluminium. Case study 2: Extrusion of aluminium.

Lecture 6 (ST)
Case study 3, 4, 5…. (useful to include a forging example, with importance of friction)

Computing classes **(ST, Terry Dickerson)**

Heat flow analysis of Jominy end-quench hardenability test, using ABAQUS.

Examples class **(HRS, ST)**

5 minute presentations of individual FE analyses of Jominy end-quench. Discussion of Examples paper problems.

COURSE MP8: BUSINESS SKILLS FOR SCIENTISTS AND ENGINEERS

[4 Lectures - Shaun Fitzgerald]

- Measures of Success
  - Financial Measures
  - Share Price Comparisons
  - Profit and Loss Accounts, Cash Flow Statements and Balance Sheets
  - Ratio Analysis
  - Quantitative Analysis (Cash Flow Analysis, Net Present Value, IRR)
  - Market Position
  - Relative Market Share/Share Growth, Competitive Market Place

- Evaluating Risk (4 lectures - Pete)

- Preparing a Business Plan (4 lectures - Shaun Fitzgerald)
  - Strategic Rationale
  - Competitive Advantage
  - Investment Requirements
  - Risk Adjusted Rate of Return
  - Team
  - Case Studies

- Managing Innovation – Organizational Structures and Culture to foster innovation (1-2 lectures – Shaun Fitzgerald)

- Communications (2-3 lectures)
  - Pyramid Principle – Answer First
  - Slide Design
  - Presentation Skills
  - Report Writing
  - Eli Lilly & Hybritech Case Study – Student seminar

COURSE MP9: NEURAL NETWORKS

[4 lectures T. Sourmail and HKDB]

Introduction {1}

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Neural Network Analysis {2}

Errors and Uncertainties {3,4}

Polymer Flow and Processing (JAE)

Lecture 1
Effect of flow fields on a polymer chain, Monte Carlo modelling. Differentiation between segmental orientation and chain extension; role of entanglements.

Case study of lattice MC modelling of liquid crystals, and the handling of fields due to microstructure, as well as variable coupling into extensional and rotational components of field.

Lecture 2
The role of disclinations and their modelling.

Case study of welding of polymers. MC lattice model showing the special structure in the region of surfaces and the relaxation of this structure to give chain interdigitation and thus weld strength.

Lecture 3
Example of multiscaling down to atomistic MD in order to time calibrate the MD as well as provide molecular detail as required.

Mould flow programs, their operation and prediction of mould filling mechanisms. Parameterisation, and extension to 3 dimensions.

Welding (HDB)

Lecture 4
Introduction to the physical metallurgy of fusion welding, the processes, technology, microstructure and properties.

Lecture 6,7
Modelling of heat flow, solidification and microstructural development from chemical compositiion and heat flow considerations. Modelling of mechanical properties. Residual Stress

COURSE MP11: MATERIAL AND PROCESS SELECTION

Leaders: Dr H R Shercliff, Dr D Cebon

AIMS

- to train graduate students in taking a systematic approach to design-led selection of materials and processes
- to develop a working knowledge of the "Cambridge Engineering Selector" software
- to introduce further approaches and software used for selection
- to apply the selection techniques via case studies

SYLLABUS

Lectures (approx. 8 hours)

- Materials Selection and Design
- Data Structure and Sources
- The CES Software
- Selection of Materials and Shape
- Advanced Methods
- Process Selection
- Building databases
- Case studies

Exercises (approx. 7 hours)

- "Teach Yourself" Tutorial in CES
- Standard Exercises (examples paper)

Course credit

Standard credit is given for completing the computing exercises and the Examples Paper.

READING MATERIAL

Ashby M.F. "*Materials selection in mechanical design*", Butterworth-Heinemann, 2nd edition, 1999. This textbook covers the selection of materials and structural sections in detail, and introduces process attributes used as the basis for process selection in the Cambridge Engineering Selector (CES) software.

Shercliff H.R. and Lovatt A.M. "*Selection of manufacturing processes in design and the role of process modelling*", to appear in Progress in Materials Science (preprints on request from hrs@eng.cam.ac.uk).

This paper reviews the problem of process selection based on process attributes, illustrating the complexity introduced by the interactions between design, material and process, and the use of process models to capture this complexity.