



MS (Part I) and MEM (Part II)  
Final Honours School  
Options Lecture Course Synopses  
2016 - 2017



Department of Materials



Materials Science (MS)  
&  
Materials, Economics and Management (MEM)

Final Honours School  
Options Lecture Course Synopses 2016-17

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## Introduction

This booklet will help you to decide which Materials Options courses to choose. It includes a synopsis and reading list for each of the options that will be taught this year.

Lecturers will also give three classes on each 12h lecture course, which will take the place of tutorials. You are required to attend the classes for the three options courses you choose for each term, unless your College tutor makes other arrangements for you. These classes will be assessed by the class teacher. He or she will grade your work and send back comments to your tutor.

MS students will take both Materials Options Papers in year 3. MEM students will take Materials Options Paper 2 in year 4. Materials Options Paper 1 (3rd year MS only) is taught entirely in Michaelmas term and Materials Options Paper 2 (3rd year MS and 4th year MEM) is taught entirely in Hilary term.

**You are advised to study three 12h lecture courses for each Materials Options paper.**

At the beginning of the third year it is possible to opt to transfer to a 3-year classified Bachelors degree. This option is intended for the rare case when a student may not wish to pursue the study of Materials Science for a further fourth year. A student opting to do this takes a smaller set of the materials option lecture courses, studying two of the 12h courses in each of Michaelmas and Hilary term rather than three.

**There are many ways in which you can arrive at a choice of options courses; it is essential to consult your College tutor who can give you advice best suited to your individual needs, abilities and interests. This booklet provides you with an overview of the syllabus of each course.**

## **M.Eng MS Candidates**

Your Part I examination in **Trinity 2017** will include two Materials Options Papers (Papers 1 and 2) based on the options courses. The Materials Options papers comprise one section for each twelve-hour Options lecture course listed in the syllabus for the paper, each section containing two questions: candidates are required to answer one question from each of any three sections and a fourth question drawn from any one of the same three sections. The total number of marks available on each options paper is 100, and all questions carry equal marks. You do not have to declare in advance which options you will attempt in the examination.

## **B.A. MS Candidates**

You will sit the same Options papers as the M.Eng candidates but will answer only two questions per paper, each from a different section, and will be allowed 1.5h for each paper. These shorter option papers will be worth 50 marks each.

## **All MS Candidates**

In addition to courses of the Materials Options Papers, 3rd year MS students are required to attend one of two Options Modules which take place during weeks 1 and 2 of Hilary Term. These modules consist of lectures, practicals and project work, and are assessed by means of coursework. A briefing on the Options Modules will be held during Michaelmas Term.

## **M.Eng MEM Candidates**

MEM Part I students are not timetabled to study any Materials Options in their third year.

The Part II examination in **Trinity 2016** will include one Materials Options Paper (Paper 2) based on the options courses to be taught in Hilary Term of your fourth year. The Materials Options papers comprise one section for each twelve-hour Options lecture course listed in the syllabus for the paper, each section containing two questions: candidates are required to answer one question from each of any three sections and a fourth question drawn from any one of the same three sections. The total number of marks available on each options paper is 100, and all questions carry equal marks. You do not have to declare in advance which options you will attempt in the examination.

## Options Paper 1

## Prediction of Materials' Properties

The objective of this option course is to introduce the students to the current state-of-the-art in first-principles materials modelling. This course develops the basic theoretical concepts underlying current computational research in materials using quantum-mechanical atomic-scale simulations. This course responds to the questions “Which materials properties can we predict using atomic-scale first principles computer simulations? How reliable are the results? How complex is the underlying methodology? What is the computational power required to perform such calculations?” This course will provide an essential background to any student willing to engage in the study of materials by combining quantum theory and high-performance computing. In addition, this course will constitute a necessary complement to the curriculum of those students oriented towards experimental materials research, as it will enable them to understand the current literature on atomistic modelling and to interact meaningfully with computational researchers throughout their future career in materials.

**Introduction to first-principles materials modelling:** Density-functional theory (DFT) and prediction of materials properties from first principles. Examples: optical absorption in silicon, superconductivity in magnesium diboride. Historical development of electronic structure calculations. Why DFT is universally adopted in quantum-mechanical atomistic modelling of materials.

**Density-functional theory I:** Many-body Schroedinger equation. Independent electron approximation. Self-consistent field method. Hartree-Fock method. Density-functional theory.

**Density-functional theory II:** Kohn-Sham representation. Exchange and correlation functionals. Electronic ground state and excited states. Limitations of density functional theory.

**Ground-state structure:** Born-Oppenheimer approximation. Atomic forces. Bulk and surface structures at zero temperature. Comparison with X-ray crystallography and Scanning Tunneling Microscopy.

**Elasticity:** Elastic constants. Predicted vs measured elastic properties. Predictions for materials under extreme conditions.

**Introduction to phonons:** Force constants and dynamical matrix. Phonons. General properties of phonon dispersion relations.

**Inelastic Neutron and X-ray scattering:** Comparison of predicted phonon dispersions to Inelastic Neutron Scattering and Inelastic X-ray Scattering measurements. Calculation of the heat capacity.

**Phonon-mediated superconductivity:** Basics of Bardeen-Cooper-Schrieffer theory. Electron-phonon coupling. Predicted critical temperatures vs experiment.

**Photoemission spectra:** Band structures. Measurement of band structures using Photoemission spectroscopy. Predicted vs measured band structures.

**Optical spectra I:** Electron-photon coupling. Direct absorption and phonon-assisted absorption.

**Optical spectra II:** Excitons. Predicted vs measured optical absorption spectra.

**Dielectric permittivity:** Lattice contribution to the dielectric screening. Predicted vs measured dielectric permittivities.

**Required reading:**

F. Giustino, **Materials modelling using density functional theory: property and predictions**, University Press, 2014

N. W. Ashcroft and N. D. Mermin, **Solid state physics**, Harcourt College Publishers, 1976

Kittel, Wiley 22KIT, **Introduction to Solid State Physics**, Ch, 6,7, 8



**Background reading:**

E. Kaxiras, **Atomic and electronic structure of solids**, Cambridge University Press, 2003

P.Y. Yu and M. Cardona, **Fundamental of semiconductors**, Springer, Heidelberg, 2003 (RSL QC 611 YU).

## **Engineering Ceramics: Synthesis & Properties**

### **1. Introduction: Engineering Ceramics**

### **2. Ceramic processing**

- Overview of ceramic processing from starting powder to final product.
- Production of powders
- Powder characterisation
- Forces between particles
- Powder processing before firing.
  - Dry forming routes.
  - Wet forming routes
- Sintering
- Reaction processing
- Sol-Gel: powderless processing of ceramics.

### **3. Mechanical properties of ceramics**

- Weibull statistics and strength of ceramics
- Time-dependent strength
- Thermal shock
- Mechanical properties and applications of:
  - a. traditional triaxial porcelains,
  - b. alumina,
  - c. zirconia,
  - d. silicon nitride,
  - e. silicon carbide.
- R-curve behaviour

**Background reading:**

**Introduction to Ceramics 2nd Ed.**, W.D. Kingery, H.K. Bowen and D.R. Uhlmann. Wiley Interscience.

**Physical ceramics : principles for ceramic science and engineering**, Yet-Ming Chiang et al., Wiley

**Sintering : densification, grain growth, and microstructure**, Suk-Joong L. Kang, Elsevier Butterworth-Heinemann (44KAN)

**Principles of Ceramic Processing 2<sup>nd</sup> Ed.**, J. S. Reed. Wiley Interscience.

**Ceramic Microstructures: Property Control by Processing** W.E. Lee and W.M. Rainforth. Chapman and Hall.

**Ceramic processing and sintering** M.N. Rahaman. 2<sup>nd</sup> edition, New York : M. Dekker, c2003 (44RAH)

**Processing of ceramics** / volume editor: Richard J. Brook, Materials science and technology (VCH) ; v. 17A & v. 17B Materials Library 44 BRO/a and b

**Engineering Materials 2**, M F Ashby and D R H Jones, Chapters 15-20.

**Mechanical Properties of Ceramics**, R W Davidge.

**Fracture of Brittle Materials**, B R Lawn.

**An Introduction to the Mechanical Properties of Ceramics**, D J Green.

**Ceramic Science for Materials Technologists**, I J McColm.

**Ceramic Microstructures**, W E Lee and W M Rainforth.

**Ceramic Matrix Composites**, I M Low (ed.).

**Toughness of Ceramics: Resistance Curves**, R I Todd, in **The Encyclopedia of Advanced Materials**, (D Bloor et al, eds.) pp. 2887-2890, Pergamon, Oxford, UK, (1994).

**Transformation Toughening**, R I Todd and M P S Saran, in **Materials Processing Handbook**, CRC Press/Taylor & Francis, Boca Raton, Florida, USA, 2007, Chapter 20.

## Strength & Failure of Materials

- **Design of strong alloys (EL):**
  - Principles of alloy design for high yield strength.
  - Examples from aluminium, titanium, nickel and iron-based alloys.
- **Fracture (EL):**
  - Plasticity and fracture.
  - Ductile - brittle transitions.
  - Principles of alloy design for high fracture strength.
  - Examples from aluminium, titanium, nickel and iron-based alloys.
- **Wear and surface treatments (EL):**
  - Wear mechanisms.
  - Wear – resistant materials.
  - Surface treatments.
- **Fatigue (AJW):**
  - Cyclic deformation of fcc, bcc & hcp metals (mostly fcc).
  - Cyclic stress strain curves.
  - Persistent slip bands, dislocation structures, strain localisation.
  - Crack initiation.
  - Crack growth.
- **Non-destructive testing (AJW):**
  - Need for NDT.
  - X-rays, ultrasonics, eddy currents, dye penetrant, magnetic particles.

**Background reading:**

**Design of strong alloys (EL):**

**Physical metallurgy**, R W Cahn & P Haasen, 1996.

**Steels: microstructure and properties**, H K D H Bhadeshia, 2006.

**Fracture (EL):**

**Fundamentals of fracture mechanics**, J F Knott, 1973.

**Fracture & ductile vs. brittle behavior**, G E Beltz (ed.), MRS Proceedings, **539**, 1999.

**Wear and surface treatments (EL):**

**Tribology**, I M Hutchings, 1992.

**Fatigue (AJW):**

**Background reading:**

**Fatigue of Materials**, S Suresh, CUP, 1991.

Fracture - 2nd year lecture notes

**Deformation & Fracture Mechanics of Engineering Materials**, R. W. Hertzberg, Wiley, 1989.

**Fatigue as a Design Criterion**, T. V. Duggan & J. Byrne, Macmillan, 1977

**Fatigue and Fracture** ASM Handbook, Vol 19

**Fundamentals of Fracture Mechanics**, J.F. Knott, Butterworths, 1975

**Fracture Mechanics—Worked Examples**, J.F. Knott & P.A. Withey, Institute of Materials, 1993

## **Materials & Devices for Optics and Optoelectronics**

1. Classical theory of light, Maxwell's equations and the wave equation. Interaction of light and matter. Snell's law. Diffraction. Refraction and reflection at interfaces. Total internal reflection. Polarization dependence.
2. Waveguides. Discrete modes of propagation. Optical fibres for telecoms. Attenuation and dispersion. Single vs multi mode fibres.
3. Birefringence and optical nonlinearity. Relevant materials. Optical switches and modulators. Wavelength conversion.
4. Novel optical materials. Photonic crystals, metamaterials
5. Semi-classical theory of light. Absorption and emission. Black body radiation and Planck's law. Einstein A and B coefficients. Electromagnetic harmonic oscillator.
6. Light emitting diodes. Inorganic and organic semiconductor devices. Wannier and Frenkel excitons. Quantum efficiency.
7. Optical amplifiers. Population inversion. Atom-like vs band engineered gain media. Semiconductor devices. Erbium doped fibres.
8. Lasers I. Optical cavities. Threshold condition for lasing. Lasing materials. Heterostructure lasers. Device designs. Quantum wells, wires, and dots.
9. Photodetection. P-i-ns, APDs, and single photon detectors.
10. Solar cells I, principles of operation
11. Solar cells II, inorganic cells. Polycrystalline silicon, single crystal heterojunction cells, and thin film semiconductor cells
12. Solar Cells III, Dye sensitized solar cells, organic solar cells and perovskites.

## Nanomaterials

### 1) Basics of nanomaterials (NG)

Nanoscale; Nanotechnology; Surface area bulk; 0-D, 1-D, 2-D materials

### 2) Synthesis of nanomaterials I (NG)

Particle synthesis chemistry, solgel; metallic nanoparticles; core-shell nanoparticles; composites, hybrid coatings, thin films

### 3) Synthesis of nanomaterials II (NG)

CVD, Arc discharge; other methods (exfoliation etc.); bulk synthesis; up-scaling; safety of nanomaterials, ethics & regulations

### 4) Carbon nanomaterials, Chalcogenides - I (NG)

Fullerenes, carbon nanotubes, graphene; sample preparation; Characterization-I methods

### 5) Carbon nanomaterials, Chalcogenides – II (KP)

Modification of carbon nanomaterials I; non-covalent; supramolecular

### 6) Modification of carbon nanomaterials II (KP)

Covalent

### 7) Characterization - II (KP)

Raman, HPLC, MS, ...

### 8) Applications of Carbon Nanomaterials (KP)

Medical; Energy

### 9) Properties at the Nanoscale (HB)

Physical properties & how they manifest at the nanoscale; challenges

### 10) Nanofabrication-I (HB)

How devices are made (optical); next steps (etching, deposition etc..)

### 11) Nanofabrication-II (HB)

AFM and E-beam-based lithography; problems with lithography

### 12) Emerging Device Concepts (HB)

Devices using nanomaterials

### Reading list:

There is no comprehensive textbook on nanomaterials. Students are encouraged to browse through the following books, as well as using the internet and reading journals, such as Nature Materials, MRS Bulletin and Nanotechnology.

### Background reading:

- **Nanostructures and Nanomaterials**, G. Cao, Imperial College Press 2004 (in RSL)
- **Nanomaterials: Synthesis, Properties and Applications**, A S Edelstein & R C Cammarata (Eds.), Taylor & Francis 1996, (DOM library: 58EDE).
- **Introduction to Nanotechnology**, C P Poole & F J Owens, Wiley, 2003, (DOM library: 58POO).
- **The Physics and Chemistry of Nanosolids**, F J Owens, C P Poole, Jr. , Wiley 2008, (DOM library: 58 OWE).
- **Introduction to Nanoscale Science and Technology**, Massimiliano Di Ventra, Kluwer, 2004 (DOM library).
- **Nanochemistry-** A chemical approach to nanomaterials, G A Ozin, A C Arsenault, L Cademartiri, RSC Publishing 2009 (DOM library: 40 OZI).
- **Introduction to Nanoscience**, G L Hornyak et al., CRC Press, Taylor & Francis 2008, (DOM library: 58 HOR/2).
- **Fundamentals of Nanotechnology**, G L Hornyak et al., CRC Press, Taylor & Francis 2008, (DOM library: 58 HOR/1).
- **Clusters and nanomaterials: theory and experiment**, Y Kawazoe, T Kondow, K Ohno (eds.) Berlin, New York: Springer, 2002 (DOM library).
- **Quantum properties of atomic-sized conductors**, N Agrait, A L Yeyati, J M van Ruitenbeek, Preprint (DOM library).
- **Nanoscale Physics for Materials Science**, T. Tsurumi, H. Hirayama, M. Vacha, T. Taniyama, CRC Press, Taylor & Francis 2010.
- **Nanophysics and Nanotechnology**. An introduction to modern concepts in nanoscience, E. L. Wolf, Wiley-VCH, 2005 (DOM library: 58 WOL/1)

### Fabrication of Nanomaterials for Materials Science Applications:

- **Nanostructured Materials: Processing, Properties and Applications**, Carl C. Koch (ed.), IOP 2002, (DOM library: 40KOC).
- **Nanostructured Materials and Nanotechnology**, Concise Edition, H.S. Nalwa (ed.), Academic Press, 2002, (DOM library: 58NAL & RSL.)



### **Carbon Nanotubes:**

- **Carbon Nanotubes and Related Structures**, P J F Harris, CUP, 1999, (**DOM library:** 40HAR.)
- **Carbon nanotubes and related structures** : synthesis, characterization, functionalization, and applications, D M Guldi and N Martin, Wiley 2010, (**DOM library:** 40 GUL)
- **Science of Fullerenes and Carbon Nanotubes**, M S Dresselhaus, G Dresselhaus, and P C Eklund, Academic Press, 1996 (**in RSL**).

### **Q-dots and Q-wires:**

- **Low-dimensional Semiconductor Structures**, K Barnham & D Vvedensky (Eds.), CUP, 2001, (**DOM library:** 21BAR.)
- **Quantum Dot Heterostructures**, D. Bimberg, Wiley 1999, (**DOM Library:** 22BIM).
- **Optical Properties of Semiconductor Quantum Dots**, U Woggon, Springer, 1997.

### **Light Scattering:**

- **Absorption and Scattering of Light by Small Crystals**, C E Bohren and D R Huffman, John Wiley, 1983.
- For surface plasmons there are two reviews that are worth reading, along with references quoted in them:  
**“Plasmonics: localization and guiding of electromagnetic energy in metal/dielectric structures”**, S Maier and H A Atwater, J. Appl. Physics, 98, 011101 (2005).  
**“Exploitation of localized surface plasmon resonance”**, E Hutter and J H Fendler, Adv. Mater., 16, 1685 (2004).

### **Environmental and safety aspects:**

- **Nanotechnology and the Environment**, editors B Karn et al, ACS Symposium Series vol 890, 2005.
- **Nanotoxicology; an emerging discipline evolving from studies of ultrafine particles**, G Oberdorster et al, Environmental Health Perspectives, 113, p823, 2005.
- **Safe Handling of nanotechnology**, A D Maynard et al, Nature, 444, p267 2006.
- **Toxicology of nanoparticles: A historical perspective**, G Oberdorster et al. Nanotoxicology, 1, p2, 2007.
- **Nanomaterials and nanoparticles: Sources and toxicity**, C Buzea et al., Biointerphases, 2, p.MR17, 2007.

## Options Paper 2

## Devices

### 1. Prof P R Wilshaw

- Semiconductor crystal growth. Purification of precursors. Czochralski and Bridgman growth. CVD, MBE.
- Fabrication of integrated circuits. Oxidation, diffusion, implantation, lithography, etching, metallization.
- Bipolar, passive, and MOS devices.
- Assembly and packaging.

#### Background reading:

**VLSI Technology**, Sze, McGraw-Hill.

**Microelectronic Materials**, Grovenor, Hilger.

**Materials for Semiconductor Devices**, Grovenor, IOM.

**Electronic Materials**, Murarka and Peckerar, Academic Press.

**Crystal Growth**, Vere, Plenum.

**VLSI Fabrication Principles**, Gandhi, Wiley.

**Electronic Materials and Devices**, Navon, Houghton/Mifflin

### 2. Prof C R M Grovenor

- Electroceramics: how to control the electrical properties of ceramics.
- Ceramic conductors: Resistors and varistors, temperature sensitive resistors, sensors and fuel cells.
- Dielectrics and capacitors: Control of permittivity, capacitor types and materials selection, dielectric memory devices.
- Piezoelectric and pyroelectric materials and devices

#### Background reading:

**Electroceramics**, A J Moulson and J M Herbert, Chapman & Hall, 1990.

**Electrical Properties of Materials**, 6th edition, Solymar and Walsh, OUP, 1998.

**Gas Sensing Materials**, MRS Bulletin, **24**, No. 6, June 1999.

### 3. Prof S C Speller

- Fundamentals of superconductivity
- Influence of microstructure on superconducting properties: flux pinning, Josephson effect.
- Superconductors for magnet applications: wires and tapes, bulks
- Superconducting thin films for device applications: digital electronics, passive microwave devices, Superconducting Quantum Interference Devices (SQUIDS).
- Novel superconducting materials. Fe based compounds.

#### Reading list:

Recommended books which are available in the Materials Library:

**Electrical Properties of Materials**, 6<sup>th</sup> edition, Solymar and Walsh, OUP, 1998, chapter 14

- Concise introduction to the fundamentals of superconductivity
- Required reading with the exception of section 14.6, which is useful as background reading

**Superconductivity**, 2<sup>nd</sup> edition, Buckel and Kleiner, Wiley-VCH, 2004

- Chapters 1-2 provide useful background information on fundamental properties and superconducting materials
- Chapters 3-6 are useful background, but the detailed mathematical treatments are beyond the scope of this course
- Chapter 7 is required reading on applications of superconductors

**High Temperature Superconductors (HTS) for Energy Applications**, Woodhead publishing, ed, Melhem, 2012

- Chapters 1-4 provide background reading on applications of HTS materials

**Concise Encyclopedia of Magnetic and Superconducting Materials**, Pergamon Press, ed Evetts, 1997

- Good reference book on a wide range of superconducting materials and applications

Other books on fundamentals of superconductivity that may be useful include:

**Superconductivity, superfluids and condensates**, Oxford Master Series in Condensed Matter Physics, Annett, 2004

- Excellent book but more advanced than needed for this course.

**Introduction to Superconductivity**, International Series in Solid State Physics, Vol 6, 2<sup>nd</sup> Rose-Innes and Rhoderick

- Undergraduate level physics book on superconductivity – not written in a very accessible style

## **Advanced Engineering Alloys & Composites: Design & Applications**

### **1. Stability of Microstructure:**

A comparison between classical nucleation and the spinodal reaction. The Cahn-Hilliard model of spinodal decomposition. Particle coarsening. Order-disorder reactions: the Bragg-Williams model. Martensitic reactions and related phenomena: e.g. bainite and shape memory effects. Crystallographic theory of martensite formation.

### **2. Design for Lightness:**

Alloys for transportation and aerospace; magnesium alloys and their applications. Advanced aluminium alloys including aluminium-lithium, aluminium-scandium, aluminium-transition metal and aluminium-transition metal-rare earth alloys. Advanced titanium alloys: near-alpha alloys, beta alloys, casting alloys. Laminates and carbon fibre composites for aerospace applications. Titanium matrix composites. Case Study: Planes, trains and automobiles.

### **3. Design for Maximum Strength and Toughness:**

High strength steels; dual phase (ferrite-martensite) steels. High-alloy tempered martensites: bearing steels and tool steels; drawn pearlitic steels; maraging steels; austempering and martempering; thermomechanical treatments: ausforming, isoforming; transformation induced plasticity (TRIP) steels. Precipitation hardened stainless steels. Case Study: aircraft undercarriages, gearboxes.

### **4. Design for High Temperatures: Superalloys and Beyond**

Creep-resistant steels; high temperature intermetallics; refractory metals: niobium, molybdenum, tantalum, tungsten, rhenium. Case Study: power generating turbines and jet engines.

**Background reading:**

**Physical Metallurgy**, 3<sup>rd</sup> edition, P Haasen, CUP, 1996, 50HAA.

**Transformations in Metals**, P G Shewmon, McGraw Hill, 1969, 53SHE.

**Fundamentals of Physical Metallurgy**, J D Verhoeven, Wiley, 1975, 50VER.

**The Theory of Transformations in Metals and Alloys**, 3rd edition, J W Christian, Pergamon, 2002, 53CHR.

**Light Alloys: From Traditional Alloys to Nanocrystals**, 4th edition, I J Polmear, Butterworth Heinemann, 2006, 52POL.

**Steels, Microstructure and Properties**, 3rd edition, H K D H Bhadeshia and R W K Honeycombe, 2005, Butterworth Heinemann, 51BHA.

**Steels : metallurgy and applications**, 2<sup>nd</sup> Edition, D.T. Llewellyn, Butterworth-Heinemann, 51LLE

**Titanium**, Gerd Lütjering, James C. Williams, Springer, 52LUT

**Selection and Use of Engineering Materials**, 3rd edition, (chapters 6-1, 15, 17, 18), J A Charles, F A A Crane & J A G Furness, Butterworth Heinemann, 1997. 56CHA.

**Structure-property relations in nonferrous metals**, Alan M. Russell, Kok Loong Lee , Wiley-Interscience, 52Rus

**Maraging steels: Modelling of microstructure, properties and applications** W Sha and Z Guo

**Creep Resistant Steels**, F.Abe

## **Advanced Manufacture with Metals & Alloys: Processing, Joining & Shaping**

### **Melt Processing - Casting & Other Melt-based Processes**

Cast iron: Grey iron, ductile iron, white iron, malleable iron.

Steel, Al alloys, metal matrix composites, Ni alloys, Ti alloys.

Grain structure, competitive growth, dendrite fragmentation, grain refiners.

Microsegregation, macrosegregation, local segregates.

Defects: porosity/pore formation, inclusions/oxide, cracks and hot tears, shrinkage, cold shuts, misruns.

Melt conditioning.

Heat flow, modelling.

Shaped casting: die casting and others.

Continuous casting: DC casting, twin roll casting, spray forming and others.

Rapid Solidification.

#### **Background reading:**

**Casting ASM Handbook Vol 15**, 9th edition, section "Principles of Solidification" and "Molding and casting processes".

**Castings**, chapters 6, 7, 8, 9 and 10, J Campbell

**Fundamentals of solidification**, chapters 2, 3, 4, 5 and 6, W Kurz and D J Fisher.

**Solidification processing**, M C Flemings.

## **Advanced Manufacture with Metals & Alloys**

### **1. Joining:**

Mechanical joining.

Soldering.

Brazing.

Welding.

Adhesive bonding.



## 2. **Surface finishing**

Cleaning.

Plating.

Coating.

Surface hardening.

### **Reading list:**

#### **Background Reading**

**N.B.** There is no single book that is required reading. There is no need to read ALL of these books – they are largely alternatives for each other – see which ones you can get hold of, or which ones suit you, but do do some reading around.

#### **Joining of Materials and Structures: From Pragmatic Process to Enabling**

**Technology**, R W Messler Jr, Elsevier Butterworth-Heinemann, 2010.

A key text covering all aspects of joining including joining a wide range of material types. (A copy has been requested for the Materials Library.)

**Manufacturing with Materials**, L Edwards and M Endean (eds.), Butterworths / Open University Press, 1990, 50MAS/4A.

The “process datacards” were taken from here. Chapter 5 covers aspects of joining.

**Process Selection: from Design to Manufacture**, 2nd edition, K G Swift and J D Booker, Butterworth-Heinemann, 2005, 56SWI.

Chapter 7 covers joining processes.

**Introduction to the Physical Metallurgy of Welding**, 2nd edition, K E Easterling, Butterworth–Heinemann, 1992, 56EAS.

A key text for understanding the materials/microstructural aspects of welding.

**Metallurgy of Welding**, 6th edition, J F Lancaster, Abington Publishing, 1999, 56LAN/B.

Covers a wide range of welding processes.

**Metals Handbook**, Desk edition, chapters 24, 26 to 30, 1985 04-1ASM (for reference only).

**Engineering Materials: Properties and Selection** 4<sup>th</sup> edition, K G Budinski, 1992, 50BUD.

Chapter 6 contains sections on polymer coatings and adhesives. Chapter 10 covers surface hardening. Chapter 19 covers inorganic coatings, including plating. (A copy of the 9<sup>th</sup> edition (2010) has been requested for the Materials Library. In this edition, the relevant chapters are Chapter 13, covering surface hardening and Chapter 21 on surface engineering.)

**Principles of Metal Manufacturing Processes**, J Beddoes and M J Bibby, 1999, Arnold, 56BED.

Chapter 9 covers surface hardening, plating and thin film coatings.

**The Superalloys**, R C Reed, 2006, Cambridge University Press, 52REE

Chapter 5 covers coatings for Ni turbine blades.

## **Biomaterials & Natural Materials**

1. Introduction to biomaterials. Definitions and history.
2. The structure and properties of natural materials.
  - a) basic building blocks - proteins, polysaccharides.
  - b) mammalian soft tissue - skin, tendon, muscle.
  - c) hard tissue -.
3. Biofunctionality.
4. Materials response to in vivo environment.  
the three classes of biomedical material:  
bioinert, bioactive and bioresorbable - the bioreactivity spectrum.
5. Tissue response to implants.
  - a) wound healing - inflammation and repair.
  - b) cellular response to implants.
6. Bioceramics, Biopolymers and Biometals and Biocomposites.
7. Tissue Engineering.
  - a) Scaffolds.
  - b) Scaffold - cell interactions.
8. Biomechanics.
  - a) the joint reaction force.
  - b) device design.
9. Drug delivery devices – liposomes, natural polymers and artificial polymer based systems.
10. Tissue expanders. Use in plastic and reconstructive surgery.
11. Osteoporosis. Trends and treatments.

### **Background reading**

**Biomaterials Science and Engineering**, 3rd edition, Park, Plenum, NY.

**Biological Performance of Materials**, J Black, Marcel Dekker, NY.

**Physiology of Bone**, 3rd edition, J Vaughan, OUP.

**An introduction to bioceramics**, L L Hench & I Wilson, eds., World Scientific.  
**Materials Science and Technology vol.14**, D F Williams (ed.), VCH, Germany.  
**Biomaterials Science, An Introduction to Materials in Medicine**, B D Rattner,  
A S Hoffman, F J Schoen and J E Lemons, Academic Press, San Diego, CA.

## Advanced Polymers

This course addresses how critical microstructural phenomena dominate the macroscopic properties of polymers, and how these are exploited in some of the more advanced polymers and 'soft materials'. This will be discussed in the context of technological and industrial applications. The course will cover:

Prof Assender (4 lectures):

- Radius of gyration and other molecular dimensions, molecules in solution and gelation
- Critical phase behavior and phase separation
- Blend and block copolymer morphology
  - Micro and nano-patterning
- Interface phenomena
  - Polymer miscibility
  - Reflectivity techniques
  - Capillary waves

Dr Telling (4 lectures):

Neutron scattering as a tool for the study of polymeric materials

1. Fundamentals of the neutron scattering technique
  - Neutron vs. X-ray vs. Light Scattering
  - Pros and cons of the two techniques
  - The neutron as a probe
  - Scattering concepts
    - Elastic and Inelastic Scattering
    - Momentum Transfer,  $Q$
    - The Scattering Process
    - Differential Cross Sections
    - Scattering Cross Sections
    - Length scales

## 2. QENS – Quasi-Elastic Neutron Scattering: The study of dynamics

- The materials scientist and polymer dynamics
- QENS : why and what
  - Coherent and Incoherent Scattering
  - Experimental Setup
  - Transmission
  - What we measure
  - Line width analysis and geometry
- Example : putting it all together

## 3. SANS – Small Angle Neutron Scattering: The study of structure

- The materials scientist and polymeric structure
- SANS : why and what
  - geometry of a SANS experiment
  - contributions to  $d\sigma/d\Omega$
  - contrast matching
  - the single particle (shape) factor,  $P(Q)$
  - the inter-particle structure factor,  $S(Q)$
  - analysis via standard plots
- Example

## 4. Recycling

- Setting the scene
- Plastic: fantastic or cheap and nasty?
- The materials life cycle: a PET bottle
- Recycling
- Recovery infrastructure

## Prof Assender (4 lectures):

- Novel molecular topologies and molecular materials
  - Molecular self-assembly
  - Drug delivery
- Understanding  $T_g$ 
  - Surface/interface  $T_g$
- Chain entanglement and reptation

- Diffusion
- Adhesion and bonding
  - Mechanical failure of polymers
- Thin film applications

**Required reading (Those books core to the course material):**

**Soft Condensed Matter**, especially chapters 2, 3 and 6 R A L Jones, OUP, 2002.  
22JON/1.

**Polymers at Surfaces and Interfaces**, R A L Jones and R W Richards, CUP, 1999.  
Chapters 4, 5, 6 & 7. 45JON/1

**Introduction to Physical Polymer Science**, 2nd edition, L H Sperling, John Wiley and Sons, 1992. Chapters 3, 5, 8 & 12. 45SPE/1

**Background reading:**

**Fundamentals of Polymer Engineering**, A Kumar and R K Gupta, McGraw-Hill, 1998.  
Chapters 9 & 13. 45KUM/1

**Polymer-Polymer Miscibility**, O Olabisi, L M Robeson and M T Shaw, Academic Press Inc, 1979. RSL QD 381.8 OLA

**Introduction to Polymer Physics**, M Doi, OUP, 1997. Chapters 2 & 5. 45DOI/1.

**The Physics of Glassy Polymers**, 2nd edition, R N Haward and R J Young (eds), Chapman and Hall, 1997. Chapters 9 & 10. RSL TA 455.P58 PHY

For lectures 5 to 8 on Neutron Methods and Recycling issues you may want to refer to the following:

- 1 **Neutron scattering: A primer**, R. Pynn, Lansce <http://library.lanl.gov/cgi-bin/getfile?00326651.pdf>
- 2 **Small angle neutron scattering**, S.M. King, ISIS Modern Techniques For Polymer Characterisation, Chapter 7, Wiley, 1999
- 3 **Quasi-Elastic Neutron Scattering**, M. Bée, Taylor & Francis, 1988, ISBN-10: 0852743718
- 4 **Materials and the environment**, M.F. Ashby Elsevier 2009, ISBN 978-1-85617-608-8

**Introduction to plastics recycling**, 2<sup>nd</sup> edition, V Goodshire, Smithers Rapra, 2007,  
Chapters 5, 8 & 9

## **Materials for Energy Production, Distribution & Storage**

### 1. Introduction.

Energy usage: domestic, transportation, industry and commerce.

Key drivers for energy supply strategy: climate change; security of resources; continuity of supply; efficiency and economy.

### 2. Electricity Production

Fossil generation: Boilers, heat exchangers, turbines, combined cycle systems

Carbon capture and storage technology

\*Nuclear fission: reactor design, fuels, cladding, moderators, cooling systems, pressure vessels, radiation damage and embrittlement, thermal ageing, stress corrosion cracking, safety systems, waste handling, treatment and storage.

\*Nuclear fusion: principles, reactor design, plasma containment, first wall materials, divertors, tritium production, latest developments.

Renewables: wind, wave, tidal, geothermal and solar thermal generation.

Biomass Technologies

\*Fuel cells: principles and practice

Hydrogen production.

### 3. Electricity Distribution

Grid design

High voltage transmission: transformers and cables

\*Superconducting transmission

### 4. Electrical Energy Storage

Pumped / pressurised energy storage systems

Superconducting storage

Supercapacitors

\*Battery technology

\*Hydrogen storage

Thermal storage systems



The course is designed to give a general overview of materials requirements for energy systems, and recent developments in this area, with more in-depth coverage of a limited number of selected topics (indicated by asterisks in the above synopsis).

#### NOTES:

- (i) Photovoltaic materials are covered in the course on semiconductor materials.
- (ii) Fossil fuel power plant materials are covered in more depth in the Advanced Engineering Alloys and Composites course.
- (iii) Composite materials for wind and wave/tidal applications can also be covered in the Advanced Engineering Alloys and Composites course if necessary.

#### Reading list:

##### Background reading:

**Sustainable Energy – Without the Hot Air**, David JC MacKay (available free at [www.withouthotair.com](http://www.withouthotair.com)). Part 1 is a gentle introduction to some of the issues in energy supply in the 21<sup>st</sup> Century, recommended as background reading.

**Energy Science: Principles, Technologies, and Impacts**, John Andrews & Nick Jelley (available at Departmental Library, shelf mark: 60 AND). A general overview of energy generation storage and transmission.

**MRS Bulletin April 2008, Vol 33, No 4**, “Harnessing Materials for Energy” (available on line at: [www.mrs.org/s\\_mrs/sec\\_subscribe.asp?CID=10867&DID=200925](http://www.mrs.org/s_mrs/sec_subscribe.asp?CID=10867&DID=200925) and at Departmental Library, shelf mark: PER). A series of articles recommended as background reading.

##### Required reading:

Conise Encyclopedia of Materials for Energy Systems, Ed. J. W. Martin

Nuclear Reactors: Coolant Materials, S.C. Chetal

Nuclear Reactors: Moderator and Reflector Materials, B.P. Sharma

Nuclear Reactors: Pressure Vessel Steels, G.R. Odette

Nuclear Reactors: Shielding Materials, M.T. Simnad

Fusion Reactors (Magnetically Confined) –Tokamaks: Materials S. Ishino.

Performance limits for fusion first-wall structural materials, D.L. Smith et al, Journal of Nuclear Materials Vol 283-287 (2000) pp. 716-720

Materials Challenges in Present and Future Wind Energy, MRS Bulletin, Vol 33 (4) (2008), pp343-354

Another Pathway to Large-Scale Power Generation: Concentrating Solar Power, MRS Bulletin, Vol 33 (4) (2008), pp364-365

Concise Encyclopedia of Materials for Energy Systems, Ed. J.W. Martin, pp 136-152, 597-599

MRS Bulletin, Harnessing Materials for Energy, Vol, 33, (4), 2008, pp 303-305, 309-315, 399-407, 411-420, 421-428

Energy Resources and Systems Volume 1: Fundamentals and Non-Renewable Resources, T.K. Ghosh and M.A. Prelas, 2009, Springer, pp 77-87, 89-122, 141-203

Elements of Thermal-Fluid System Design, L.C. Burmeister, 1998, Prentice Hall, pp74-108

PEM Fuel Cells: Theory and Practice, F. Barbir, 2005, Elsevier, pp 1-31

Energy Storage, R. A. Higgins, 2010, Springer, pp 69-92

Thermal Energy Storage: Systems and Applications, I Dincer, M. Rosens, 2011, Wiley, pp 83-290

Fundamentals of electrochemical capacitor design and operation, J.R. Miller, P. Simon, 2008, The Interface, ECS Publications, pp 31-32

Nanotechnology for the Energy Challenge, J. Garcia-Martinez, 2010, Wiley-VCH, pp 139-153

Battery Technology Handbook, A. Kiehne, 2003, Verlag, pp 1-111

Electric Power Generation, Transmission, And Distribution, Leonard L. Grigsby, 2007, CRC Press, Chapters, 8, 9, 11, 13,14,19

The Smart Grid: Enabling Energy Efficiency and Demand Response, Clark W. Gellings, 2009, The Farmont Press, pp 1-14

## Options Modules

The two week block at the beginning of Hilary Term is set aside for intensive practical work. There will be two choices for the block: **Modelling of Materials**, and **Characterisation of Materials**. Students need to sign up to either of the two week practical blocks by the end of 8th week of Michaelmas Term. There will be a pre-sign up meeting in 7th week of Michaelmas Term, to allow time to make a decision about which option to take. The sign up procedure will be coordinated through the Director of Studies.

Options Module

Weeks 1 & 2, Hilary Term

3rd year MS

Prof M Castell (& others)

Two weeks of lectures, guided practicals, and independent practical work

## **Advanced Characterisation of Materials**

### **Week 1 Monday – Thursday:**

Lectures and guided practicals for each experimental technique are given. On the morning of the Thursday sample sets are chosen and instrument time is booked.

### **Week 1 Thursday – Week 2 Friday:**

This period will be devoted to independent practical work and preparation of the project report.

### **Means of examination:**

Each student will write a project report (2000-3000 words), which will be marked by the assessors out of a maximum of 50 marks. The reports will be handed in by midday Tuesday of week 3, Hilary Term. A model report will be available to provide some guidance. Attendance at all lectures and guided practicals is a compulsory requirement for the booking of instrument time.

## Introduction to Modelling in Materials Science

Lectures and hands-on practical classes.

### Synopsis:

1. Introduction to multiscale modelling and scientific computing: hierarchies in materials modelling, basic methodologies, example applications; introduction to Unix/Linux, and graphical and mathematical software.
2. Electronic modelling: modern approach using density functional theory (DFT), effective one-electron Schrödinger equation, exchange and correlation energy; plane waves versus localized basis set methodologies; applications including STM images, EELS spectra, heat of formation and elastic moduli.
3. Atomistic modelling: interatomic potentials for ionic, covalent, metallic and biological systems; molecular dynamics (MD) simulations, fundamental concepts and algorithms; applications including pair correlation functions in amorphous materials, defect evolution in irradiated metals, and growth of semiconductor films.
4. Microstructural modelling: coarse-grained atomic degrees of freedom, transition state theory, lattice gas models; Monte Carlo (MC) and kinetic Monte Carlo (kMC) simulations, fundamental concepts and algorithms; applications including order in alloys, diffusion and chemical reactions.
5. Continuum modelling: finite element method (FEM), fundamental concepts and algorithms; applications including heat flow, fluid flow and solid mechanics.

### Assessment:

Each student will write a combined report (2000-3000 words) on two mini-projects, which will be marked by the assessors out of a maximum of 50 marks. The reports will be handed in by midday Tuesday of week 3, Hilary Term.

**Background reading:**

**Introduction to materials modelling**, Barber, Maney, 2005, 12BAR.

**Learning the Unix operating system**, Peek, Todino and Strang, 12PEE.

**The mathematica book**, Wolfram, CUP, 2005, 10WOL.

**A chemist's guide to density functional theory**, Koch and Holthausen, Wiley, 2001, 40KOC.

**Electronic structure: basic theory and practical methods**, Martin, CUP, 2004, MAR21.

**Bonding and structure of molecules and solids**, Pettifor, OUP, 1995, 22PET.

**Understanding molecular simulation: from algorithms to applications**, Frenkel and Smit, Academic Press, 2002, 12FRE.

**Computer simulation of liquids**, Allen and Tildesley, OUP, 1987, 12ALL.

**The finite element method**, Pepper and Heinrich, Taylor & Francis, 2005, 10PEP.



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