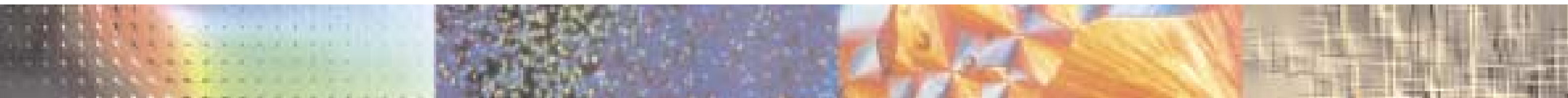
Oxford Materials

Materials Science
Final Honours School
Options Lecture Course Synopses
2019-20



Department of Materials

Materials Science (MS)

Final Honours School

Options Lecture Course Synopses 2019-20

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 up to 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: Materials Options Paper 1 is taught entirely in Michaelmas term and Materials Options Paper 2 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 2020** 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.

Options Paper 1

Options Paper 1 Michaelmas Term

Dr C.E. Patrick

12 lectures

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.

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.

Optical spectra II: Direct absorption and phonon-assisted absorption.

Excitons: Predicted vs measured optical absorption spectra.

Background Reading

Recommended course textbook:

Materials Modelling using Density Functional Theory: Properties and Predictions, F. Giustino, Oxford University Press, 2014

Additional references, especially for information on superconductivity and photoemission:

Solid state physics, N. W. Ashcroft and N. D. Mermin, Harcourt College Publishers, 1976 chapter 34

Solid state physics: An Introduction to Principles of Materials Science, H Ibach and H Luth, Springer, 2009, chaps 7 and 10

Other electronic structure references:

Introduction to Solid State Physics, C. Kittel, Wiley 22KIT, chaps 6, 7, 8

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

Fundamentals of semiconductors, P. Y. Yu and M. Cardona, Springer, 2003

Options Paper 1 Michaelmas Term

Prof R.I. Todd

12 lectures

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

Riley, F.L., **Structural Ceramics: Fundamentals and Case Studies**, CUP

Kingery, W.D., Bowen, H.K., & Uhlmann, D.R., **Introduction to Ceramics**, Wiley Interscience

Chiang, Y. M., et al., **Physical ceramics: principles for ceramic science and engineering**, Wiley

Kang, S. L., Sintering: **densification, grain growth, and microstructure**, Elsevier Butterworth-Heinemann

Reed, J.S., **Principles of Ceramic Processing**, Wiley Interscience

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

Rahaman, M.N., **Ceramic processing and sintering**, M. Dekker

Brook, R.J., **Processing of ceramics**, VCH

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

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

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

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

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

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

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

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

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

Options Paper 1 Michaelmas Term

Prof J.M. Smith

12 lectures

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 nolinearity. 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.

Required Reading

Fox, M., **Optical properties of solids**, Oxford University Press, An excellent overview of the materials properties and some basic devices

Background Reading

Hecht, E., **Optics**, Addison Wesley. A standard undergraduate text in optics

Wilson, J. & Hawkes, J., **Optoelectronics: and introduction**, Prentice Hall. A good introduction to some of the devices featured

Singh J, **Optoelectronics**, McGraw Hill. A good introduction to some of the devices featured

Senior, **Optical Fiber Communications**, Prentice Hall. A standard text on fibre communications

Rogers, A., **Essentials of Optoelectronics**, Chapman and Hall. A good introduction to some of the devices featured

Nelson, J., **The physics of solar cells**, Imperial College Press. A good introduction to solar cells

Options Paper 1 Michaelmas Term

Prof N. Grobert, Prof K. Porfyrakis & Prof H. Bhaskaran

12 lectures

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

Cao, G., **Nanostructures and Nanomaterials**, Imperial College Press

Edelstein, A. S. & Cammarata, R. C., eds., **Nanomaterials: Synthesis, Properties and Applications**, Taylor & Francis, DOM library: 58EDE

Poole, C. P., & Owens, F. J., **Introduction to Nanotechnology**, Wiley, DOM library: 58POO

Owens, F. J., & Poole, C. P., **The Physics and Chemistry of Nanosolids**, Wiley, DOM library: 58 OWE

Di Ventra, M., **Introduction to Nanoscale Science and Technology**, Kluwer, DOM library

Ozin, G.A., Arsenault, A. C., & Cademartiri, L., **Nanochemistry- A chemical approach to nanomaterials**, RSC Publishing, DOM library: 40 OZI

Hornyak, G.L., et al., **Introduction to Nanoscience**, CRC Press, Taylor & Francis, DOM library: 58 HOR/2

Kawazoe, Y., Kondow, T., & Ohno, K., eds., **Clusters and nanomaterials: theory and experiment**, Springer, DOM library

Agrait, N., Yeyati, A. L., & van Ruitenbeek, J. M., **Quantum properties of atomic-sized conductors**, Preprint, DOM library

Tsurumi, T., Hirayama, H., Vacha, M., & Taniyama, T., **Nanoscale Physics for Materials Science**, CRC Press, Taylor & Francis

Wolf, E. L., **Nanophysics and Nanotechnology. An introduction to modern concepts in nanoscience**, Wiley-VCH, DOM library: 58 WOL/1

Madou, M. J., **Fundamentals of Microfabrication and Nanotechnology**, 3 volumes, CRC Press

Fabrication of Nanomaterials for Materials Science Applications

Koch, K. C., ed., **Nanostructured Materials: Processing, Properties and Applications**, IOP, DOM library: 40KOC

Nalwa, H. S., ed**., Nanostructured Materials and Nanotechnology**, Concise Edition, Academic Press, DOM library: 58NAL & RSL

Carbon Nanotubes

Harris, P. J. F., **Carbon Nanotubes and Related Structures**, Cambridge University Press, DOM library: 40HAR

Guldi, D.M., & Martin, N., **Carbon nanotubes and related structures: synthesis, characterization, functionalization, and applications**, Wiley, DOM library: 40 GUL

Dresselhaus, M.S., Dresselhaus, G. & Eklund, P.C., **Science of Fullerenes and Carbon Nanotubes**, Academic Press

Q-dots and Q-wires

Barnham, K., & Vvedensky, D., eds., **Low-dimensional Semiconductor Structures**, Cambridge Univeristy Press, DOM library: 21BAR

Bimberg, D., **Quantum Dot Heterostructures**, Wiley, DOM Library: 22BIM

Woggon, U., **Optical Properties of Semiconductor Quantum Dots**, Springer

Light Scattering

Bohren, C.E., & Huffman, D. R., **Absorption and Scattering of Light by Small Crystals**, Wiley

For surface plasmons there are two reviews that are worth reading, along with references quoted in them:

> Maier, S., & Atwater, H. A., **"Plasmonics: localization and guiding of electromagnetic energy in metal/dielectric structures**" in J. Appl. Physics, 98, 011101.
>
> Hutter, E. & Fendler, J. H., **"Exploitation of localized surface plasmon resonance"**, in Adv. Mater., 16, 1685

Environmental and safety aspects

Karn, B., et al. eds., **Nanotechnology and the Environment**, Vol. 890, ACS Symposium Series

Oberdorster, G., et al., **Nanotoxicology; an emerging discipline evolving from studies of ultrafine particles**, in Environmental Health Perspectives, 113, p823

Maynard, A. D., et al., **Safe Handling of nanotechnology**, in Nature, 444, p267,

Oberdorster, G., et al., **Toxicology of nanoparticles: A historical perspective, in Nanotoxicology**, 1, p. 2.

C Buzea et al., **Nanomaterials and nanoparticles: Sources and toxicity**, in Biointerphases, 2, p.MR17

Options Paper 1 Michaelmas Term

Prof K.A.Q. O'Reilly & Dr E. Liotti

12 lectures

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, Melt Processing - Casting & Other Melt-based Processes: section "Principles of Solidification" and "Molding and casting processes"

Campbell, J., **Castings**, Melt Processing - Casting & Other Melt-based Processes: chapters 6, 7, 8, 9 and 10

Kurz, W., & Fisher, D. J., **Fundamentals of solidification**, Melt Processing - Casting & Other Melt-based Processes: chapters 2, 3, 4, 5 and 6

Flemings, M. C., **Solidification processing**, Melt Processing - Casting & Other Melt-based Processes

Advanced Manufacture with Metals & Alloys

1. **Joining:**
    - Mechanical joining.
    - Soldering.
    - Brazing.
    - Welding.
    - Adhesive bonding.
2. **Surface finishing**
    - Cleaning.
    - Plating.
    - Coating.
    - Surface hardening.

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.

Messler, R. W., Jr., **Joining of Materials and Structures: From Pragmatic Process to Enabling Technology**, Elsevier Butterworth-Heinemann. 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.)

Edwards, L., & Endean, M., eds., **Manufacturing with Materials**, Butterworths / Open University Press. 50MAS/4A. The "process datacards" were taken from here. Chapter 5 covers aspects of joining.

Swift, K. G. & Booker, J. D., **Process Selection: from Design to Manufacture**, Butterworth Heinemann. 56SWI. Chapter 7 covers joining processes.

Easterling, K. E., **Introduction to the Physical Metallurgy of Welding**, Butterworth Heinemann. 56EAS. A key text for understanding the materials/microstructural aspects of welding.

Lancaster, J. F., **Metallurgy of Welding**, and Abington Publishing, 56LAN/B. Covers a wide range of welding processes.

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

Budinski, K. G., **Engineering Materials: Properties and Selection**, 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 9th 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.)

Beddoes, J., & Bibby, M. J., **Principles of Metal Manufacturing Processes**, Arnold, 56BED. Chapter 9 covers surface hardening, plating and thin film coatings.

Reed, R. C., **The Superalloys**, Cambridge University Press, 52REE. Chapter 5 covers coatings for Ni turbine blades

Options Paper 2

Options Paper 2 Hilary Term

Prof C.R.M. Grovenor, Prof S.C. Speller & Prof P.R. Wilshaw

12 lectures

Devices

1. 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

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

Solymar, & Walsh, **Electrical Properties of Materials**, Oxford University Press, Gas Sensing Materials, in MRS Bulletin,

Solymar, & Walsh, **Electrical Properties of Materials**, Oxford University Press chapter 14. Concise introduction to the fundamentals of superconductivity. Required reading with the exception of section 14.6, which is useful as background reading

2. 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.

Recommended books which are available in the Materials Library:

Solymar, & Walsh, **Electrical Properties of Materials**, Oxford University Press, chapter 14. Concise introduction to the fundamentals of superconductivity. **Required reading** with the exception of section 14.6, which is useful as background reading

Buckel, & Kleiner, **Superconductivity**, Wiley-VCH. Chapter 7 is **required reading** on applications of superconductors

Buckel, & Kleiner, **Superconductivity**, Wiley-VCH. 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.
Melhem, ed., **High Temperature Superconductors (HTS) for Energy Applications**, Woodhead Publishing
Evetts, ed., **Concise Encyclopedia of Magnetic and Superconducting Materials**, Pergamon. Good reference book on a wide range of superconducting materials and applications

Other books on fundamentals of superconductivity that may be useful include:
Annett, **Superconductivity, superfluids and condensates**, Oxford Master Series in Condensed Matter Physics. Excellent book but more advanced than needed for this course.
Rose-Innes, & Rhoderick, **Introduction to Superconductivity**, International Series in Solid State Physics, Vol 6, Undergraduate level physics book on superconductivity – not written in a very accessible style.

3. 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

Sze, S. M., **VLSI Technology**, McGraw-Hill
Grovenor, **Microelectronic Materials**, Hilger
Grovenor, **Materials for Semiconductor Devices**, IOM
Murarka, & Peckerar, **Electronic Materials**, Academic Press
Vere, **Crystal Growth**, Plenum Press
Ghandhi, **VLSI Fabrication Principles**, Wiley
Navon, **Electronic Materials and Devices**, Houghton/Mifflin

Options Paper 2 Hilary Term

Prof M.L. Galano & Prof D.E.J. Armstrong

12 lectures

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 decompostion. 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

Hassan, P., **Physical Metallurgy**, Cambridge University Press, 50HAA

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

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

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

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

Bhadeshia, H. K. D. H., & Honeycombe, R. W. K., Steels, **Microstructure and Properties**, Butterworth Heinemann, 51BHA

Llewellyn, D.T., **Steels: metallurgy and applications**, Butterworth Heinemann, 51LLE

Lütjering, G., & Williams, J. C., Titanium, Springer, 52LUT

Charles, J. A., Crane, F. A. A., & Furness, J. A. G., **Selection and Use of Engineering Materials**, Butterworth Heinemann, 56CHA. Chapters 6-1, 15, 17, 18

Russell, A. M., & Lee, K. L., **Structure-property relations in nonferrous metals**, Wiley-Interscience, 52Rus

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

Abe, F., **Creep Resistant Steels**

Options Paper 2 Hilary Term

Prof J.T. Czernuszka

12 lectures

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

Park, **Biomaterials Science and Engineering**, Plenum Press

Black, J., **Biological Performance of Materials**, Marcel Decker

Vaughan, J., **Physiology of Bone**, Oxford University Press

Hench, L. L., & Wilson, I., eds., **An introduction to bioceramics**, World Scientific

Williams, D. F., ed., **Materials Science and Technology** vol.14, VCH

Rattner, B. D., Hoffman, A. S., Schoen, F. J., & Lemons, J. E., **Biomaterials Science, An Introduction to Materials in Medicine**, Academic Press

Options Paper 2 Hilary Term

Prof H.E. Assender & Dr M. Lefferts

12 Lectures

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 (8 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
- 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

Dr Lefferts (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

Required Reading

Jones, R. A. L., **Soft Condensed Matter**, Oxford University Press especially chapters 2, 3 and 6

Jones, R. A. L., & Richards, R. W., **Polymers at Surfaces and Interfaces**, Cambridge University Press, Chapters 4, 5, 6 & 7

Sperling, L. H., Introduction to Physical Polymer Science, Wiley, Chapters 3, 5, 8 & 12

Background Reading

Kumar, A., & Gupta, R. K., **Fundamentals of Polymer Engineering**, Marcel Dekker Chapter 13

Olabisi, O., Robeson, L. M., & Shaw, M. T., **Polymer-Polymer Miscibility**, Academic Press

Doi, M., **Introduction to Polymer Physics**, Oxford University Press, Chapters 2 & 5

Haward, R. N., & Young, R. J., eds., **The Physics of Glassy Polymers**, Chapman and Hall, Chapters 9 & 10

For lectures on Neutron Methods and Recycling issues:

Pynn, R., **Neutron scattering: A primer**, Lansce http://library.lanl.gov/cgi-bin/getfile?00326651.pdf.

King, S. M., **Small angle neutron scattering**, Wiley, Chapter 7 ISIS Modern Techniques For Polymer Characterisation

Bée, M., **Quasi-Elastic Neutron Scattering**, Taylor & Francis

Ashby, M. F., **Materials and the environment**, Elsevier

Goodshire, V., **Introduction to plastics recycling**, Smithers Rapra, Chapters 5, 8 & 9

Options Paper 2 Hilary Term

Prof T.J. Marrow & Dr P. Adamson

12 lectures

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.

Required Reading

Martin, J. W., ed., **Concise Encyclopedia of Materials for Energy Systems**, Elsevier, http://solo.bodleian.ox.ac.uk/primo-explore/fulldisplay?docid=oxfaleph017062013&context=L&vid=SOLO&search_scope=LSCOP_ALL&tab=local&lang=en_US

Chetal, S. C., Nuclear Reactors: Coolant Materials

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

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

Simnad, M. T., Nuclear Reactors: Shielding Materials

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

Smith, D.L., et al., **Performance limits for fusion first-wall structural materials'**, in Journal of Nuclear Materials, pp. 716-720, http://solo.bodleian.ox.ac.uk/primo-explore/fulldisplay?docid=TN_sciversesciencedirect_elsevierS0022-3115(00)00315-9&context=PC&vid=SOLO&search_scope=LSCOP_ALL&tab=local&lang=en_US

Hayman, B et al, **Materials Challenges in Present and Future Wind Energy**, in MRS Bulletin, pp. 343-354, http://solo.bodleian.ox.ac.uk/primo-explore/fulldisplay?docid=TN_crossref10.1557/mrs2008.70&context=PC&vid=SOLO&search_scope=LSCOP_ALL&tab=local&lang=en_US

Mehos, M, **Another Pathway to Large-Scale Power Generation: Concentrating Solar Power in MRS Bulletin**, pp. 364-365, http://solo.bodleian.ox.ac.uk/primo-explore/fulldisplay?docid=TN_crossref10.1557/mrs2008.72&context=PC&vid=SOLO&search_scope=LSCOP_ALL&tab=local&lang=en_US

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

Arunachalam, V. S. & Fleischer, Elizabeth L., MRS Bulletin, **Harnessing Materials for Energy**, MRS, pp. 303-305, 309-315, 399-407, 411-420, 421-428

Ghosh, T.K., & Prelas, M.A. , **Energy Resources and Systems Volume 1: Fundamentals and Non-Renewable Resources**, Springer, pp. 77-87, 89-122, 141-203, http://solo.bodleian.ox.ac.uk/primo-explore/fulldisplay?docid=oxfaleph017561997&context=L&vid=SOLO&search_scope=LSCOP_ALL&tab=local&lang=en_US

Burmeister, L.C., **Elements of Thermal-Fluid System Design**, Prentice Hall, pp. 74-108

Barbir, F., PEM Fuel Cells: Theory and Practice, Elsevier, pp. 1-31 Electronic Resource, http://solo.bodleian.ox.ac.uk/primo-explore/fulldisplay?docid=oxfaleph000496097&context=L&vid=SOLO&search_scope=LSCOP_ALL&isFrbr=true&tab=local&lang=en_US

Huggins, R. A., **Energy Storage**, Springer pp. 69-92, http://solo.bodleian.ox.ac.uk/primo-explore/fulldisplay?docid=oxfaleph021338336&context=L&vid=SOLO&search_scope=LSCOP_ALL&isFrbr=true&tab=local&lang=en_US

Dincer, I., Rosens, M., **Thermal Energy Storage: Systems and Applications**, Wliey pp. 83-290, http://solo.bodleian.ox.ac.uk/primo-explore/fulldisplay?docid=oxfaleph000532433&context=L&vid=SOLO&search_scope=LSCOP_ALL&isFrbr=true&tab=local&lang=en_US

Miller, J.R., & Simon, P., **Fundamentals of electrochemical capacitor design and operation, The Interface**, ECS Publications, pp. 31-32, https://www.electrochem.org/dl/interface/spr/spr08/spr08_p31-32.pdf

Garcia-Martinez, J., **Nanotechnology for the Energy Challenge**, Wiley-VCH. pp. 139-153, http://solo.bodleian.ox.ac.uk/primo-explore/fulldisplay?docid=oxfaleph017209467&context=L&vid=SOLO&search_scope=LSCOP_ALL&isFrbr=true&tab=local&lang=en_US

Kiehne, A., **Battery Technology Handbook**, Verlag, pp. 1-111, http://solo.bodleian.ox.ac.uk/primo-explore/fulldisplay?docid=oxfaleph019468882&context=L&vid=SOLO&search_scope=LSCOP_ALL&tab=local&lang=en_US

Grigsby, L. L., **Electric Power Generation, Transmission, And Distribution**, CRC Press Chapters 8, 9, 11, 13,14,19, http://solo.bodleian.ox.ac.uk/primo-explore/fulldisplay?docid=oxfaleph016571831&context=L&vid=SOLO&search_scope=LSCOP_ALL&isFrbr=true&tab=local&lang=en_US

Gellings, C. W., **The Smart Grid: Enabling Energy Efficiency and Demand Response**, The Farmont Press, pp. 1-14, electronic resource, http://solo.bodleian.ox.ac.uk/primo-explore/fulldisplay?docid=oxfaleph000623896&context=L&vid=SOLO&search_scope=LSCOP_ALL&tab=local&lang=en_US

Background Reading

MacKay, D. J. C., **Sustainable Energy – Without the Hot Air**, available free at www.withouthotair.com. Part 1 is a gentle introduction to some of the issues in energy supply in the 21st Century, recommended as background reading, http://solo.bodleian.ox.ac.uk/primo-explore/fulldisplay?docid=TN_dspace1810/217849&context=PC&vid=SOLO&search_scope=LSCOP_ALL&tab=local&lang=en_US

Andrews, J., & Jelley, N., **Energy Science: Principles, Technologies, and Impacts**, OUP, A general overview of energy generation storage and transmission. http://solo.bodleian.ox.ac.uk/primo-explore/fulldisplay?docid=oxfaleph019489577&context=L&vid=SOLO&search_scope=LSCOP_ALL&isFrbr=true&tab=local&lang=en_US

Arunachalam, V. S. & Fleischer, Elizabeth L., **'Harnessing Materials for Energy'** in MRS Bulletin, MRS, available on line at: http://solo.bodleian.ox.ac.uk/primo-explore/fulldisplay?docid=TN_untlark/67531/metadc894448&context=PC&vid=SOLO&search_scope=LSCOP_ALL&tab=local&lang=en_US and at Departmental Library, shelf mark: PER). A series of articles recommended as background reading

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: **Introduction to Modelling of Materials**, and **Advanced 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 5th 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

Prof M.P. Moody (& 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.

Options Module Weeks 1 & 2, Hilary Term

Prof R. Drautz & Prof J.R. Yates

One week of lectures and practicals, one week of project work

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:

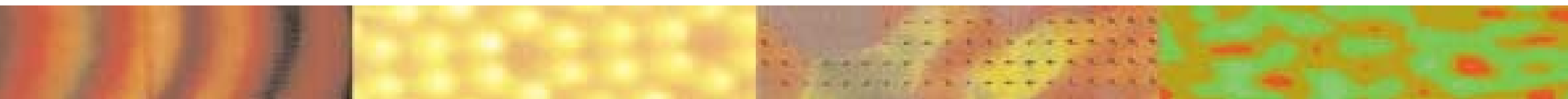
Each student will write a combined report (2000-3000 words) on two mini-projects, which will be marked by the assessors out of a maximum of 50 marks. The reports will be handed in by midday Tuesday of week 3, Hilary Term.

Background Reading

Barber, & Maney, **Introduction to materials modelling**

Feliciano Giustino, **Materials Modelling using Density Functional Theory**, OUP

Martin, **Electronic structure: basic theory and practical methods**, Cambridge University Press
Frenkel, & Smit, **Understanding molecular simulation: from algorithms to applications**, Academic Press
Allen, & Tildesley, **Computer simulation of liquids**, Oxford University Press   Both editions ok.
Pepper, & Heinrich, **The finite element method**, Taylor & Francis



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