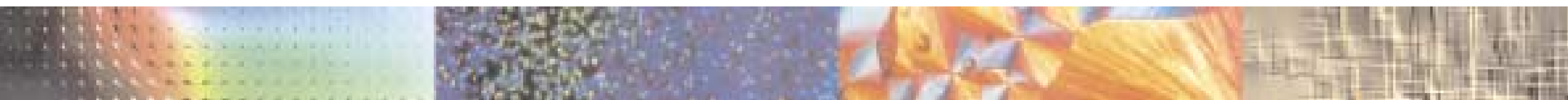
OxfordMaterials

Materials Science
Final Honours School
Options Lecture Course Synopses
2020-21



Department of Materials

Materials Science (MS)

Final Honours School

Options Lecture Course Synopses 2020-21

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.

Students will take both Materials Options Papers in year 3: Materials Options Paper 1 is taught in Michaelmas term and Materials Options Paper 2 is taught in Hilary term.

You are advised to study <u>three</u> 12h lecture courses for <u>each</u> 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. Candidates

Your Part I examination in **Trinity 2021** 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. 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 Candidates

In addition to courses of the Materials Options Papers, 3rd year students are required to attend the Introduction to Modelling in Materials Science module in week 6 of Michaelmas Term, and one of two Options Modules which take place during weeks 4 and 5 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 early in Hilary 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 and addresses 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?" This course will provide an essential background to any student interested in learning how a combination of quantum theory and high-performance computing allows materials to be studied computationally "from first principles", that is, without using empirical models. This course is also appropriate for students more 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. 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.

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

Measurement of phonon properties: Comparison of predicted phonon dispersions to experimental measurements.

Magnetic properties: Concepts of spin density and magnetization. The Stoner criterion and exchange splitting. Ferro/ferri/antiferromagnetic ground states.

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

Optical spectra I: Electron-photon coupling and calculation of the dielectric function.

Optical spectra II: Direct absorption and phonon-assisted absorption. Different models of excitons.

Background reading

Ashcroft, Neil W. and N. David Mermin. **Solid State Physics**. Holt, Rinehart & Winston, 1976. Dept. of Materials Library 22 ASH/C.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph010079933

Giustino, Feliciano. **Materials Modelling Using Density Functional Theory : Properties and Predictions.** Oxford University Press, 2014. Dept. of Materials Library 10 GIU.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph019717301

Ibach, H. and H. Lüth. **Solid-State Physics : An Introduction to Principles of Materials Science**. Springer Berlin Heidelberg : Imprint: Springer, 2009. Online.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph020357382

Kaxiras, Efthimios. **Atomic and Electronic Structure of Solids.** Cambridge University Press, 2003. Dept. of Materials Library 22 KAX.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph015471658

Kohanoff, Jorge. **Electronic Structure Calculations for Solids and Molecules : Theory and Computational Methods.** Cambridge University Press, 2006. Electronic Structure Calculations for Solids & Molecules. Online.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph001385103

Martin, Richard M. **Electronic Structure : Basic Theory and Practical Methods.** Cambridge University Press, 2004. Cambridge Core. online.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph021836066

Yu, Peter Y. and Manuel Cardona. **Fundamentals of Semiconductors : Physics and Materials Properties.** Springer Berlin Heidelberg : Imprint: Springer, 2010. Graduate Texts in Physics. Online.
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph020357475

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

Ashby, M. F. and David R. H. Jones. **Engineering Materials 2 : An Introduction to Microstructures and Processing.** 4th edition, Butterworth-Heinemann, 2013. Dept. of Materials Library 50 ASH/5.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph019438244 Chapters 15-20

Bloor, D. and R. W. Cahn. **The Encyclopedia of Advanced Materials**. Pergamon, 1994. Dept. of Materials Library 01 BLO/a (REFERENCE).
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph011088061 Toughness of Ceramics: Resistance Curves in The Encyclopedia of Advanced Materials, Bloor, D. et al, eds.) pp. 2887-2890.

Brook, R. J. **Processing of Ceramics.** VCH, 1996. Materials Science and Technology (Vch) ; V. 17a & V. 17b. Dept. of Materials Library 01 MST/17A (REFERENCE).
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph011668089

Chiang, Yet-ming et al. **Physical Ceramics : Principles for Ceramic Science and Engineering.** Wiley, 1996. Mit Series in Materials Science and Engineering. Dept. of Materials Library 44 CHI.
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph012254337

Dailly, D. F. "**Mechnical Properties of Ceramics:** R.W. Davidge, Cambridge University Press, U.K. 1979 (£ 15) (Paperback 1980 £ 3.95) 165pp." vol. 1, 1980, pp. 175-175. doi:10.1016/0142-9612(80)90045-9;
http://solo.bodleian.ox.ac.uk/permalink/f/1lj314/TN_elsevier_sdoi_10_1016_0142_9612_80_90045_9.

Green, D. J. **An Introduction to the Mechanical Properties of Ceramics.** Cambridge University Press, 1998. Cambridge Solid State Science Series.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph013324827

Groza, Joanna R. **Materials Processing Handbook.** CRC Press/Taylor & Francis, 2007. Dept. of Materials Library 04-1 GRO.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph016255405 Chapter 20.

Kang, S. J. L. **Sintering [Electronic Resource] : Densification, Grain Growth, and Microstructure.** Elsevier Butterworth-Heinemann, 2005. Ebook Central.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph000503876

Lawn, Brian R. **Fracture of Brittle Solids.** 2nd edition, Cambridge University Press, 1993. Cambridge Solid State Science Series. Dept. of Materials Library 54 LAW.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph010832070

Lee, W. E. and W. Mark Rainforth. **Ceramic Microstructures : Property Control by Processing.** Chapman & Hall, 1994. Dept. of Materials Library 44 LEE.
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph011109315

Low, It-Meng. **Ceramic Matrix Composites : Microstructure, Properties and Applications.** CRC Press ; Woodhead Publishing, 2006. Woodhead Publishing in Materials. Dept. of Materials Library 44 LOW.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph016038830

McColm, I. J. **Ceramic Science for Materials Technologists**. Leonard Hill, 1983.
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph010698484

Rahaman, M. N. **Ceramic Processing and Sintering.** 2nd edition, M. Dekker, 2003. Materials Engineering (Marcel Dekker, Inc.) ; 23. Dept. of Materials Library 44 RAH.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph015964165

Reed, James Stalford. **Principles of Ceramics Processing.** 2nd edition, Wiley, 1995. Dept. of Materials Library Overnight 44 REE.
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph011670258

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, Mark. **Optical Properties of Solids.** Second edition, Oxford University Press, 2010. Oxford Master Series in Condensed Matter Physics. Online.
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph000783472

An excellent overview of the materials properties and some basic devices.

Background reading

Hecht, Eugene. **Optics.** Fifth edition. Global edition, Pearson Education Limited, 2017. Ebook Central. online.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph021907724
A standard undergraduate text in optics.

Nelson, Jenny. **The Physics of Solar Cells.** Imperial College Press, 2003. Dept. of Materials Library 21 NEL.
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph015644171
A good introduction to solar cells.

Rogers, A. J. **Essentials of Optoelectronics : With Applications.** Chapman & Hall, 1997. Optical and Quantum Electronics Series ; 4.
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph013288058
A good introduction to some of the devices featured.

Senior, John M. **Optical Fiber Communications : Principles and Practice.** 3rd edition, Prentice Hall, 2009. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph016743142
A standard text on fibre communications.

Singh, Jasprit. **Optoelectronics : An Introduction to Materials and Devices**. McGraw-Hill, 1996. Mcgraw-Hill Series in Electrical and Computer Engineering.
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph012395575
A good introduction to some of the devices featured.

Wilson, J. and J. F. B. Hawkes. **Optoelectronics : An Introduction.** 3rd edition, Prentice Hall Europe, 1998. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph013133791
A good introduction to some of the devices featured.

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; Characterisation-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) **Characterisation - 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

Background reading

Agraït, Nicolás et al. **"Quantum Properties of Atomic-Sized Conductors."** Physics reports, vol. 377, no. 2-3, 2003, pp. 81-279, doi:10.1016/S0370-1573(02)00633-6. http://solo.bodleian.ox.ac.uk/permalink/f/1lj314/TN_elsevier_sdoi_10_1016_S0370_1573_02_00633_6

Andrew, D. Maynard et al. **"Safe Handling of Nanotechnology."** Nature, vol. 444, no. 7117, 2006, p. 267, doi:10.1038/444267a.
http://solo.bodleian.ox.ac.uk/permalink/f/1lj314/TN_nature_a10.1038/444267a
Environmental and safety aspects.

Barnham, Keith and Dimitri D. Vvedensky. **Low-Dimensional Semiconductor Structures : Fundamentals and Device Applications.** Cambridge University Press, 2001. Dept. of Materials Library 21 BAR.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph015150579 Q-dots and Q-wires.

Bimberg, Dieter et al. **Quantum Dot Heterostructures.** John Wiley, 1999. Dept. of Materials Library Overnight 22 BIM.
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph013595393 Q-dots and Q-wires.

Bohren, Craig F. and Donald R. Huffman. **Absorption and Scattering of Light by Small Particles.** Wiley, 1983.
http://solo.bodleian.ox.ac.uk/permalink/f/n9grc9/oxfaleph021472649 Light Scattering.

Buzea, C. et al. **"Nanomaterials and Nanoparticles: Sources and Toxicity."** Biointerphases, vol. 2, no. 4, 2007, pp. MR17-MR71, doi:10.1116/1.2815690.
http://solo.bodleian.ox.ac.uk/permalink/f/1lj314/TN_wos000256467100002 Environmental and safety aspects.

Cao, Guozhong. **Nanostructures & Nanomaterials : Synthesis, Properties & Applications.** Imperial College Press, 2004. Nanostructures and Nanomaterials.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph015707053

Di Ventra, Massimiliano et al. **Introduction to Nanoscale Science and Technology.** Kluwer Academic Publishers, 2004. Nanoscale Science and Technology. Dept. of Materials Library Overnight 58 DIV.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph015775045

Dresselhaus, M. S. et al. **Science of Fullerenes and Carbon Nanotubes.** Academic Press, 1996. http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph012040977 Carbon Nanotubes.

Edelstein, A. S. and R. C. Cammarata. **Nanomaterials : Synthesis, Properties, and Applications.** Institute of Physics Publishing, 1996. Dept. of Materials Library 58 EDE. http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph012260293.

Guldi, D. M. **Carbon Nanotubes and Related Structures [Electronic Resource] : Synthesis, Characterization, Functionalization, and Applications.** Wiley-VCH Verlag, 2010. Online. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph021932221 Carbon Nanotubes

Harris, Peter J. F. **Carbon Nanotubes and Related Structures : New Materials for the Twenty-First Century.** Cambridge University Press, 1999. Dept. of Materials Library 40 HAR. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph013713486 Carbon Nanotubes

Hornyak, Gabor L. **Introduction to Nanoscience.** CRC ; Taylor & Francis [distributor], 2008. Dept. of Materials Library 58 HOR/2. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph017083668

Hutter, E. and J. H Fendler. **"Exploitation of Localized Surface Plasmon Resonance." Advanced Materials,** vol. 16, no. 19, 2004, pp. 1685-1706, doi:10.1002/adma.200400271. http://solo.bodleian.ox.ac.uk/permalink/f/1lj314/TN_wj10.1002/adma.200400271 Light Scattering. For surface plasmons there are two reviews that are worth reading, along with references quoted in them

Karn, Barbara. **Nanotechnology and the Environment : Applications and Implications.** American Chemical Society, 2005. Acs Symposium Series ; 890. Dept. of Materials Library Overnight 05 ACS/2005. http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph015887193 Environmental and safety aspects.

Kawazoe, Y, editor et al. **Clusters and Nanomaterials : Theory and Experiment.** 1st ed. 2002. edition, Springer Berlin Heidelberg : Imprint: Springer, 2002. Springer Series in Cluster Physics. Online. http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph021933955

Koch, C. C. **Nanostructured Materials: Processing, Properties, and Applications.** 2nd edition, William Andrew Pub., 2007. Materials Science and Process Technology Series. Dept. of Materials Library Overnight 40 KOC. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph021934000 Fabrication of Nanomaterials for Materials Science Applications.

Madou, Marc J. **Fundamentals of Microfabrication and Nanotechnology.** Volume Iii : From Mems to Bio-Mems and Bio-Nems : Manufacturing Techniques and Applications. Third edition, CRC Press, 2011. Ebook Central. Online.

http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph001089444 Environmental and safety aspects.
Maier, Stefan A. and Harry A. Atwater. **"Plasmonics: Localization and Guiding of Electromagnetic Energy in Metal/Dielectric Structures."** Journal of Applied Physics, vol. 98, no. 1, 2005, doi:10.1063/1.1951057.
http://solo.bodleian.ox.ac.uk/permalink/f/1lj314/TN_aip_complete10.1063/1.1951057 Light Scattering. For surface plasmons there are two reviews that are worth reading, along with references quoted in them.
Nalwa, Hari Singh. **Nanostructured Materials and Nanotechnology.** Concise edition, Academic Press, 2002. Dept. of Materials Library 58 NAL REFERENCE.
http://solo.bodleian.ox.ac.uk/permalink/f/n9grc9/oxfaleph015198980 Fabrication of Nanomaterials for Materials Science Applications.
Oberdorster, G. et al. **"Nanotoxicology: An Emerging Discipline Evolving from Studies of Ultrafine Particles."** Environ. Health Perspect., vol. 113, 2005, pp. 823-839. doi:10.1289/ehp.7339;
http://solo.bodleian.ox.ac.uk/permalink/f/1lj314/TN_wos000230250800028. Environmental and safety aspects.
Oberdörster, Günter et al. **"Toxicology of Nanoparticles: A Historical Perspective."** Nanotoxicology, vol. 1, no. 1, 2007, pp. 2-25, doi:10.1080/17435390701314761.
http://solo.bodleian.ox.ac.uk/permalink/f/1lj314/TN_informaworld_s10_1080_17435390701314761 Environmental and safety aspects.
Owens, Frank J. and Charles P. Poole. **The Physics and Chemistry of Nanosolids.** Wiley-Interscience, 2008. Dept. of Materials Library Overnight 58 OWE.
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph016918681
Ozin, Geoffrey A. et al. **Nanochemistry : A Chemical Approach to Nanomaterials.** 2nd edition, Royal Society of Chemistry, 2009. Dept. of Materials Library 40 OZI/1.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph016915487
Poole, Charles P. and Frank J. Owens. **Introduction to Nanotechnology**. Wiley-Interscience, 2003. Dept. of Materials Library Overnight 58 POO.
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph015553599.
Tsurumi, Takaaki. **Nanoscale Physics for Materials Science.** CRC Press, 2010. Taylor & Francis Ebooks. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph021928785
Woggon, Ulrike. **Optical Properties of Semiconductor Quantum Dots.** Springer, 1997. Springer Tracts in Modern Physics ; 136.
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph019706221 Q-dots and Q-wires.

Wolf, Edward L. **Nanophysics and Nanotechnology : An Introduction to Modern Concepts in Nanoscience.** Third edition, Wiley-VCH, 2015. Ebook Central. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph000868476 DOM library: 58 WOL/1**.**

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.

Advanced Manufacture with Metals & Alloys

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

Background reading

Beddoes, Jonathan and M. J. Bibby. **Principles of Metal Manufacturing Processes**. Arnold, 1999. Dept. of Materials Library 56 BED. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph013776691 Joining & Surface finishing: 56BED. Chapter 9 covers surface hardening, plating and thin film coatings.

Budinski, Kenneth G. **Engineering Materials : Properties and Selection.** 4th edition, Prentice Hall, 1992. Dept. of Materials Library 50 BUD. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph016576121 Joining & Surface finishing: 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.).

Campbell, John. **Castings.** 2nd edition, Butterworth-Heinemann, 2003. Dept. of Materials Library 56 CAM/1. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph015518436 Melt Processing - Casting & Other Melt-based Processes: chapters 6, 7, 8, 9 and 10.

Davis, J. R. **Metals Handbook**. Desk ed., 2nd edition, ASM International, 1998. Dept. of Materials Library 04-1 ASM/DESK (REFERENCE). http://solo.bodleian.ox.ac.uk/permalink/f/n9grc9/oxfaleph013669097 Joining & Surface finishing: chapters 24, 26 to 30, 1985 04-1ASM (for reference only)

Easterling, K. E. **Introduction to the Physical Metallurgy of Welding.** 2nd edition, Butterworth-Heinemann, 1992. Dept. of Materials Library 56 EAS/1. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph010700152 Joining & Surface finishing: 56EAS. A key text for understanding the materials/microstructural aspects of welding.

Edwards, Lyndon and Mark Endean. **Manufacturing with Materials.** Open University Press ; Butterworths, 1990. Materials in Action Series. Dept. of Materials Library 50 MAS/4B. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph010423981 Joining & Surface finishing: 50MAS/4A. The “process datacards” were taken from here. Chapter 5 covers aspects of joining.

Flemings, Merton C. **Solidification Processing.** McGraw-Hill, 1974. Mcgraw-Hill Series in Materials Science and Engineering. Dept. of Materials Library 53 FLE/B.

http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph010393983 Melt Processing - Casting & Other Melt-based Processes.
Kurz, Wilfried and D. J. Fisher. **Fundamentals of Solidification.** 4th revised edition, Trans Tech, 1998. Dept. of Materials Library 53 KUR.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph013239251 Melt Processing - Casting & Other Melt-based Processes: chapters 2, 3, 4, 5 and 6.
Lancaster, J. F. **Metallurgy of Welding.** 6th edition, Abington, 1999. Dept. of Materials Library 56 LAN/B. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph013762706 Joining & Surface finishing: Covers a wide range of welding processes.
Messler, Robert W. **Joining of Materials and Structures: From Pragmatic Process to Enabling Technology**. Elsevier Butterworth-Heinemann, 2004. Dept. of Materials Library Overnight 54 MES. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph017279322 Joining & Surface finishing: 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.)
Reed, Roger C. **The Superalloys : Fundamentals and Applications.** Cambridge University Press, 2006. Dept. of Materials Library 52 REE.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph016106716 Joining & Surface finishing: Chapter 5 covers coatings for Ni turbine blades.
Swift, K. G. and J. D. Booker. **Process Selection: From Design to Manufacture**. 2nd edition, Butterworth-Heinemann, 2003. Dept. of Materials Overnight 56 SWI.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph015717437 Joining & Surface finishing: Chapter 7 covers joining processes.

Options Paper 2

Top

Options Paper 2 Hilary Term

Prof P. Wilshaw, Prof S.C. Speller and tbc

12 lectures

Devices

1. tbc

- Electroceramics: how to control the electrical properties of ceramics; doping and control of resistivity
- 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 materials and devices

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.

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.

Required reading

Buckel, Werner et al. **Superconductivity : Fundamentals and Applications.** 2nd ed., rev. and enlarg edition, Wiley-VCH, 2004. Dept. of Materials Library Overnight 21 BUC/A.

http://solo.bodleian.ox.ac.uk/primo-explore/fulldisplay?docid=oxfaleph015489386&context=L&vid=SOLO&search_scope=LSCOP_ALL&isFrbr=true&tab=local&lang=en_US Chapter 7 is required reading on applications of superconductors

Solymar, L. and D. Walsh. **Electrical Properties of Materials.** 6th edition, Oxford University Press, 1998. Materials Dept. Library 21 SOL/Q. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph013048023 chapter 14. Concise introduction to the fundamentals of superconductivity. Required reading with the exception of section 14.6, which is useful as background reading

Background reading

Annett, James F. **Superconductivity, Superfluids, and Condensates**. Oxford University Press, 2004. Oxford Master Series in Condensed Matter Physics. http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph015533956 Excellent book but more advanced than needed for this course.

Buckel, Werner et al. **Superconductivity : Fundamentals and Applications.** 2nd ed., rev. and enlarg edition, Wiley-VCH, 2004. Dept. of Materials Library Overnight 21 BUC/A. http://solo.bodleian.ox.ac.uk/primo-explore/fulldisplay?docid=oxfaleph015489386&context=L&vid=SOLO&search_scope=LSCOP_ALL&isFrbr=true&tab=local&lang=en_US 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.

Evetts, J. et al. **Concise Encyclopedia of Magnetic & Superconducting Materials.** Pergamon, 1992. Advances in Materials Science and Engineering. Dept. of Materials Library 21 EVE. http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph010604338 Good reference book on a wide range of superconducting materials and applications.

Grovenor, C. **Materials for Semiconductor Devices.** Institute of Metals, 1987. Book (Institute of Metals); 360. Dept. of Materials Library 21 GRO/C. http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph010855781

Grovenor, C. **Microelectronic Materials.** Adam Hilger, 1989. Graduate Student Series in Materials Science and Engineering. Dept. of Materials Library 21 GRO/1A. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph010203763

Melhem, Ziad. **High Temperature Superconductors (Hts) for Energy Applications.** Woodhead Publishing, 2012. Woodhead Publishing in Energy ; No. 27. Dept. of Materials

Library Overnight 21 MEL.
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph019302654

Moulson, A. J. and J. M. Herbert. **Electroceramics : Materials, Properties, Applications.** Chapman and Hall, 1990. Dept. of Materials Library 44 MOU/B.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph010334942

Murarka, S. P. and Martin Charles Peckerar. **Electronic Materials : Science and Technology.** Academic Press, 1989.
http://solo.bodleian.ox.ac.uk/permalink/f/n9grc9/oxfaleph010808471

Navon, David H. **Electronic Materials and Devices.** Houghton Mifflin, 1975.
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph012913580

Rose-Innes, Alistair Christopher and E. H. Rhoderick. **Introduction to Superconductivity**. 2d edition, Pergamon Press, 1978. International Series in Solid State Physics ; V. 6. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph021836597
Undergraduate level physics book on superconductivity – not written in a very accessible style.

Solymar, L. and D. Walsh. **Electrical Properties of Materials**. 6th edition, Oxford University Press, 1998. Materials Dept. Library 21 SOL/Q.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph013048023

Sze, S. M. **Vlsi Technology**. 2nd edition, McGraw-Hill, 1988. Mcgraw-Hill Series in Electrical Engineering. Dept. of Materials Library Overnight 21 SZE/3.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph010022837

Vere, A. W. **Crystal Growth : Principles and Progress**. Plenum, 1987. Updates in Applied Physics and Electrical Technology. Dept. of Materials Library Overnight 30 VER.
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph010030729

Watson, J. et al. **"Gas-Sensing Materials."** MRS Bulletin, vol. 24, no. 6, 1999, pp. 14-15, doi:10.1557/S0883769400052453.
http://solo.bodleian.ox.ac.uk/permalink/f/1lj314/TN_scopus2-s2.0-0033148263 article in MRS Bulletin vol. 24, iss. 6, pp. 14-17.

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

Abe, Fujio et al. **Creep-Resistant Steels.** Woodhead Publishing, 2008. Woodhead Publishing in Materials. Dept. of Materials Library 54 ABE. http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph017292662

Bhadeshia, H. K. D. H. and R. W. K. **Honeycombe. Steels : Microstructure and Properties.** 3rd edition, Butterworth Heinemann, 2006. Dept. of Materials Library 51 BHA. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph000496200

Christian, J. W. **The Theory of Transformations in Metals and Alloys**. 3rd edition, Pergamon, 2002. Ebook Central. Dept. of Materials Library 53CHR. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph000985500

Crane, F A A et al. **Selection and Use of Engineering Materials.** 3rd edition, Elsevier Science, 1997. Ebook Central. http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph000504724 56CHA. Chapters 6-1, 15, 17, 18.

Leyens, C. and M. Peters. **Titanium and Titanium Alloys : Fundamentals and Applications.** Wiley-VCH, 2003. Dept. of Materials Library 52 LEY. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph015647538

Llewellyn, David T. **Steels : Metallurgy and Applications.** 2nd edition, Butterworth-Heinemann, 1994. Dept. of Materials Library 51 LLE/A. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph011084310

Lütjering, G. and J. C. Williams. **Titanium.** Springer, 2003. Engineering Materials and Processes. Dept. of Materials Overnight 52 LUT. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph015971137

Polmear, I. J. Light Alloys : **From Traditional Alloys to Nanocrystals.** Fourth edition, Elsevier Butterworth-Heinemann, 2006. Dept. of Materials Library 52 POL/J. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph016043150

Russell, Alan M. and Kok Loong Lee. **Structure-Property Relations in Nonferrous Metals**. Wiley-Interscience, 2005. Dept. of Materials Library Overnight 52 RUS. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph015973222

Sha, Wei and Zhanli Guo. **Maraging Steels : Modelling of Microstructure, Properties and Applications**. CRC ; Woodhead, 2009. Dept. of Materials Library Overnight 50 SHA. http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph017144317

Verhoeven, John D. **Fundamentals of Physical Metallurgy.** Wiley, 1975. Dept. of Materials Library 50 VER/B. http://solo.bodleian.ox.ac.uk/primo-

explore/fulldisplay?docid=oxfaleph010194928&context=L&vid=SOLO&search_scope=LSCOP_ALL&tab=local&lang=en_US

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.

Required / Background Reading

Black, Jonathan. **Biological Performance of Materials : Fundamentals of Biocompatibility.** 3rd ed., rev. and expand edition, Marcel Dekker, 1999. Dept of Materials Library 45 BLA.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph015260336 This 3rd revised edition specified.
---. **Biological Performance of Materials : Fundamentals of Biocompatibility**. 4th edition, Taylor & Francis, 2006. online.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph016020876 This is not the specified edition; but the latest one with ebook.

Hench, Larry L. **An Introduction to Bioceramics.** Second edition, Imperial College Press, 2013. Online. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph019706215 This is not the specified edition; but the latest one with ebook.

Hench, Larry L. and June Badeni**. An Introduction to Bioceramics**. World Scientific, 1993. Advanced Series in Ceramics ; Vol. 1. Dept of Materials Library 44 HEN.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph011019892 This edition specified.

Park, Joon Bu. **Biomaterials Science and Engineering.** Plenum, 1984. Dept of Materials Library 45 PAR. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph010765235

Ratner, B. D. et al. **Biomaterials Science : An Introduction to Materials in Medicine**. Third edition, Elsevier : Academic Press, 2013. Online.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph019706218 This 3rd edition specified.

Vaughan, Janet. **The Physiology of Bone**. Third edition, Clarendon Press, 1981. Oxford Science Publications. Online.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph010192681 This 3rd edition specified.

Williams, D. F**. Medical and Dental Materials**. VCH, 1992. Materials Science and Technology (Vch) ; V. 14. Dept of Materials Library 01 MST/14 and online.
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph010639616

Options Paper 2 Hilary Term

Prof H.E. Assender & Dr M.J. 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, Richard A. L. and R. W. Richards. **Polymers at Surfaces and Interfaces.** Cambridge University Press, 1999. Dept. of Materials Library Overnight 45 JON/1. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph013676033 Chapters 4, 5, 6 & 7.

Sperling, L. H. **Introduction to Physical Polymer Science.** 2nd edition, Wiley, 1992. Wiley-Interscience Publication. Dept. of Materials Library 45 SPE/1. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph010645237 Chapters 3, 5, 8 & 12.

Background reading

Ashby, M. F. **Materials and the Environment : Eco-Informed Material Choice.** Elsevier Butterworth-Heinemann, 2009. Dept. of Materials Library 57 ASH. http://solo.bodleian.ox.ac.uk/primo-explore/fulldisplay?docid=oxfaleph016971177&context=L&vid=SOLO&search_scope=LSCOP_ALL&isFrbr=true&tab=local&lang=en_US For lectures 5 to 8 on Neutron Methods and Recycling issues.

Bée, M. **Quasielastic Neutron Scattering : Principles and Applications in Solid State Chemistry, Biology, and Materials Science**. Adam Hilger, 1988. http://solo.bodleian.ox.ac.uk/permalink/f/n9grc9/oxfaleph010022488 For lectures 5 to 8 on Neutron Methods and Recycling issues.

Doi, M. **Introduction to Polymer Physics.** Clarendon Press, 1996. Oxford Science Publications. Dept. of Materials Library 45 DOI/1. http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph011703032 Chapters 2 & 5.

Goodship, Vannessa. **Introduction to Plastics Recycling.** 2nd edition, Smithers Rapra, 2007. Dept. of Materials Library Overnight 57 GOO. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph017062988 Chapters 5, 8 & 9.

Jones, Richard A. L. **Soft Condensed Matter.** Oxford University Press, 2002. Oxford Master Series in Condensed Matter Physics ; 6. Dept. of Materials Library 22 JON/1. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph015357928 especially chapters 2, 3 and 6

Kumar, Anil and Rakesh K. Gupta. **Fundamentals of Polymer Engineering.** Second edition, revised and expand edition, Marcel Dekker, 2003. Plastics Engineering (Marcel Dekker, Inc.) ; 66. Dept. of Materials Library 45 KUM/1. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph016131691 Chapter 13.

Olabisi, Olagoke et al. **Polymer-Polymer Miscibility.** Academic Press, 1979. http://solo.bodleian.ox.ac.uk/primo-explore/fulldisplay?docid=oxfaleph012916260&context=L&vid=SOLO&search_scope=LSCOP_ALL&tab=local&lang=en_US

Pethrick, R. A. and J. V. Dawkins. **Modern Techniques for Polymer Characterisation.** Wiley, 1999. http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph013579849 For lectures 5 to 8 on Neutron Methods and Recycling issues. Chapter 7 ISIS Modern Techniques For Polymer Characterisation.

Pynn, R. . **"Neutron Scattering: A Primer."** http://library.lanl.gov/cgi-bin/getfile?00326651.pdf http://library.lanl.gov/cgi-bin/getfile?00326651.pdf For lectures 5 to 8 on Neutron Methods and Recycling issues.

Young, Robert J. and Robert Nobbs Haward. **The Physics of Glassy Polymers**. 2nd ed edition, Chapman & Hall, 1997. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph013362915 Chapters 9 & 10.

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

Arunachalam, V. S. and E. L. Fleischer. **"Harnessing Materials for Energy."** MRS Bulletin, vol. 33, no. 4, 2008, pp. 261-261, doi:10.1557/mrs2008.60. http://solo.bodleian.ox.ac.uk/permalink/f/1lj314/TN_crossref10.1557/mrs2008.60 pp. 303-305, 309-315, 399-407, 411-420, 421-428.

Deng, Da. **"Li-Ion Batteries: Basics, Progress, and Challenges."** vol. 3, 2015, pp. 385-418. doi:10.1002/ese3.95; http://solo.bodleian.ox.ac.uk/permalink/f/1lj314/TN_wj10.1002/ese3.95. Vol 3: 385-418

Gellings, Clark W. **The Smart Grid : Enabling Energy Efficiency and Demand Response.** Fairmont Press, 2009. Ebook Central. http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph000623896 pages 1-14.

Ghosh, Tushar K, author and Mark A Prelas. **Energy Resources and Systems** : Volume 1: Fundamentals and Non-Renewable Resources. 1st ed. 2009. edition, Springer Netherlands : Imprint: Springer, 2009. http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph021933930 pp. 77-87, 89-122, 141-203.

Grigsby, Leonard L. **Electric Power Generation, Transmission, and Distribution**. 3rd edition, CRC Press, 2012. Electrical Engineering Handbook Series. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph001084806 chapters 8, 9, 14, 19

Hayman, Brian et al. **"Materials Challenges in Present and Future Wind Energy."** MRS Bulletin, vol. 33, no. 4, 2008, pp. 343-353, doi:10.1557/mrs2008.70. http://solo.bodleian.ox.ac.uk/permalink/f/1lj314/TN_crossref10.1557/mrs2008.70 pp. 343-354.

Mehos, Mark. **"Another Pathway to Large-Scale Power Generation: Concentrating Solar Power."** MRS Bulletin, vol. 33, no. 4, 2008, pp. 364-366, doi:10.1557/mrs2008.72. http://solo.bodleian.ox.ac.uk/permalink/f/1lj314/TN_crossref10.1557/mrs2008.72 pp. 364-365.

Miller, J. R. and P. Simon. **"Fundamentals of Electrochemical Capacitor Design and Operation."** Electrochemical Society Interface, vol. 17, no. 1, 2008, pp. 31-32, http://solo.bodleian.ox.ac.uk/permalink/f/1lj314/TN_scopus2-s2.0-48249120989. pp. 31-32.

Smith, D. L. et al. **"Performance Limits for Fusion First-Wall Structural Materials."** Journal of nuclear materials, vol. 283-287, no. I, 2000, pp. 716-720, doi:10.1016/S0022-3115(00)00315-9.
http://solo.bodleian.ox.ac.uk/permalink/f/1lj314/TN_elsevier_sdoi_10_1016_S0022_3115_00_00315_9 pp. 716-720.

Stork, D. and S. J. Zinkle. **"Introduction to the Special Issue on the Technical Status of Materials for a Fusion Reactor."** Nuclear Fusion, vol. 57, no. 9, 2017, p. 092001, doi:10.1088/1741-4326/aa69e4.
http://solo.bodleian.ox.ac.uk/permalink/f/1lj314/TN_iop10.1088/1741-4326/aa69e4

Background reading

Andrews, John and N. A. Jelley. **Energy Science : Principles, Technologies, and Impacts.** Second edition, Oxford University Press, 2013.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph019489577

Burmeister, Louis C. **Elements of Thermal-Fluid System Design.** Prentice Hall, 1998.
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph021726139

Charit, Inajit and K. Linga Murty. **An Introduction to Nuclear Materials : Fundamentals and Applications.** Wiley-VCH, 2013.
http://solo.bodleian.ox.ac.uk/permalink/f/89vilt/oxfaleph021406027

Dinçer, İbrahim and Marc Rosen. **Thermal Energy Storage [Electronic Resource]: Systems and Applications.** 2nd edition, Wiley, 2010. Ebook Central.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph000532433

Elliott, David. **Energy Storage Systems.** 2017. Physics World Discovery, publisher Institute of Physics.
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MacKay, David. **Sustainable Energy - without the Hot Air.** UIT Cambridge, 2009.
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McDonald, Andre G. and Hugh L. Magande. **Introduction to Thermo-Fluids Systems Design.** Wiley, 2012. Ebook Central.
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Coursework Modules

In week 6 of Michaelmas Term, all students will take the Introduction to Modelling in Materials Science module, followed by a period of self-study supported by the Demonstrators via ‘surgeries’. A two week block in weeks 4 and 5 of Hilary Term is set aside for intensive practical work. There will be two choices for this block: **Atomistic Modelling**, and **Advanced Characterisation of Materials**. Students need to sign up to either of the two week practical blocks by the end of the 2nd week of Hilary Term. There will be a pre-sign up meeting in week 8 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 Undergraduate Studies.

Compulsory Module | Week 6, Michaelmas Term

Prof R. Drautz, Prof J.R. Yates & Prof E. Tarleton

One week of lectures and practicals + “surgeries”

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 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 25 marks. The reports will be handed in by midday Tuesday of the week following Michaelmas Term (namely, 9^{th} week).

Background reading

Allen, M. P. and D. J. Tildesley. **Computer Simulation of Liquids.** Clarendon Press, 1989. Dept. of Materials Library 12 ALL. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph010203993 Both editions ok.

Dunne, Fionn and Nik Petrinic. **Introduction to Computational Plasticity.** Oxford University Press, 2005. Ebook Central. http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph000514503

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Options Module Weeks 4 & 5, Hilary Term

Prof M.P. Moody, Prof. M.L. Galano & Prof. N. Grobert

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

Advanced Characterisation of Materials

The aim of this course is to ensure a good practical grasp of core characterisation methods, introduce selected advanced microscopy techniques and to become acquainted with research facilities in the Department. This will provide an introduction to independent planning of an experimental campaign. In the first week lectures will be given on the theory and practical application of characterization techniques including: optical microscopy, scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD), scanning transmission electron microscopy (STEM), electron energy loss spectroscopy (EELS), electron backscatter diffraction (EBSD), secondary ion mass spectroscopy (SIMS) and atom probe tomography (APT). The remaining period will be devoted to independent research and preparation of the project report.

Means of examination:

Each student will write a project report (3000 words), which will be marked by the assessors out of a maximum of 25 marks. The reports will be submitted by midday Tuesday of week 6, Hilary Term. A model report will be available to provide some guidance.

Options Module   Weeks 4 & 5, Hilary Term

Dr C.E. Patrick and Prof. J. R. Yates

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

Atomistic Modelling

“Atomistic modelling” refers to the understanding of materials in terms of the individual atoms that they are made up of. Being able to predict how different atoms interact with each other requires a quantum mechanical approach, and density-functional theory (DFT) is a hugely popular theoretical framework developed for this purpose. The aim of this module is that students gain competency in setting up, running, and analysing the results of DFT calculations, including the ability to critically assess the reliability of their results. These skills are useful not just for computational materials scientists, but also experimentalists, who are increasingly taking advantage of the widespread availability of user-friendly DFT software to help interpret their results.

The first week consists of lectures and guided exercises designed to give the students the necessary skills required to be able to calculate a range of materials properties within DFT. The second week consists of independent project work where the students perform a computational “characterisation” of a material, i.e. planning, setting up and running calculations to study the properties of a given material, and then analysing the obtained results.

Means of examination:

Each student will write a project report (max. 3000 words) describing their computational characterisation, which will be marked by the assessors out of a maximum of 25 marks. The projects will be assigned at the end of the first week to be completed autonomously during the second week, with reports due in by midday Tuesday of week 6, Hilary Term.

Background reading

Giustino, Feliciano. **Materials Modelling Using Density Functional Theory : Properties and Predictions.** Oxford University Press, 2014. Dept. of Materials Library 10 GIU.
http://solo.bodleian.ox.ac.uk/permalink/f/n28kah/oxfaleph019717301

Hafner, Jürgen. **"Ab-Initio Simulations of Materials Using Vasp: Density-Functional Theory and Beyond."** Journal of Computational Chemistry, vol. 29, no. 13, 2008, pp.

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Martin, Richard M. **Electronic Structure : Basic Theory and Practical Methods.** Cambridge University Press, 2004. Cambridge Core. online.
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