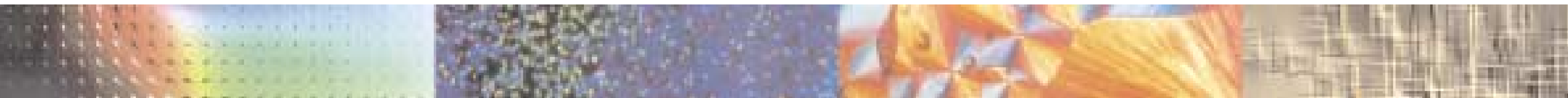
DEPARTMENT OF MATERIALS

Materials Science
Options Lecture Course Synopses
2023-24



Department of Materials

Materials Science (MS)

Final Honours School

Options Lecture Course Synopses 2023-24

Version	Action	Date
Version 1.0	Published in MT23	03/10/2023

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. They 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 2024** 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 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 towards the end of Michaelmas Term.

Options Paper 1

Top

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.

Further reading

Ashcroft, Neil W. and N. David Mermin. **Solid State Physics**. Holt, Rinehart & Winston, 1976. Dept. of Materials Library 22 ASH/C.

Giustino, Feliciano. **Materials Modelling Using Density Functional Theory: Properties and Predictions.** Oxford University Press, 2014. Dept. of Materials Library 10 GIU.

Ibach, H. and H. Lüth. **Solid-State Physics: An Introduction to Principles of Materials Science**. Springer Berlin Heidelberg: Imprint: Springer, 2009. Online.

Kaxiras, Efthimios. **Atomic and Electronic Structure of Solids.** Cambridge University Press, 2003. Dept. of Materials Library 22 KAX.

Kohanoff, Jorge. **Electronic Structure Calculations for Solids and Molecules: Theory and Computational Methods.** Cambridge University Press, 2006. Electronic Structure Calculations for Solids & Molecules. Online.

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

Yu, Peter Y. and Manuel Cardona. **Fundamentals of Semiconductors: Physics and Materials Properties.** Springer Berlin Heidelberg: Imprint: Springer, 2010. Graduate Texts in Physics. Online.

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

Further 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. Chapters 15-20 .

Bloor, D. and R. W. Cahn. **The Encyclopedia of Advanced Materials**. Pergamon, 1994. Dept. of Materials Library 01 BLO/a (REFERENCE). 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.

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.

Dailly, D. F. "**Mechnical Properties of Ceramics:** R.W. Davidge, Cambridge University Press, U.K. 1979) 165pp." vol. 1, 1980, pp. 175-175.

Green, D. J. **An Introduction to the Mechanical Properties of Ceramics.** Cambridge University Press, 1998. Cambridge Solid State Science Series.

Groza, Joanna R. **Materials Processing Handbook.** CRC Press/Taylor & Francis, 2007. Dept. of Materials Library 04-1 GRO. Chapter 20.

Kang, S. J. L. **Sintering [Electronic Resource] : Densification, Grain Growth, and Microstructure.** Elsevier Butterworth-Heinemann, 2005. Ebook Central.

Kingery, W. D. et al. **Introduction to Ceramics**. 2nd edition, John Wiley & Sons, 1976. Wiley Series on the Science and Technology of Materials.

Lawn, Brian R. **Fracture of Brittle Solids.** 2nd edition, Cambridge University Press, 1993. Cambridge Solid State Science Series. Dept. of Materials Library 54 LAW.

Lee, W. E. and W. Mark Rainforth. **Ceramic Microstructures : Property Control by Processing.** Chapman & Hall, 1994. Dept. of Materials Library 44 LEE.

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.

McColm, I. J. **Ceramic Science for Materials Technologists**. Leonard Hill, 1983.

Rahaman, M. N. **Ceramic Processing and Sintering.** 2nd edition, M. Dekker, 2003. Materials Engineering (Marcel Dekker, Inc.); 23. Dept. of Materials Library 44 RAH.

Reed, James Stalford. **Principles of Ceramics Processing.** 2nd edition, Wiley, 1995. Dept. of Materials Library Overnight 44 REE.

Options Paper 1 Michaelmas Term

Dr S. Olakkil Veedu and Prof A.A.R. Watt

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.

Further reading

Boyd, Robert W. **Nonlinear Optics**. 3rd edition, Academic Press, 2008. Includes bibliographical references and index.

Fox, Mark. **Optical Properties of Solids.** Second edition, Oxford University Press, 2010. Oxford Master Series in Condensed Matter Physics. Online. An excellent overview of the materials properties and some basic devices.

Hecht, Eugene. **Optics.** Fifth edition. Global edition, Pearson Education Limited, 2017. Ebook Central. online. A standard undergraduate text in optics.

Nelson, Jenny. **The Physics of Solar Cells.** Imperial College Press, 2003. Dept. of Materials Library 21 NEL. A good introduction to solar cells.

Rogers, A. J. **Essentials of Optoelectronics: With Applications.** Chapman & Hall, 1997. Optical and Quantum Electronics Series; 4. A good introduction to some of the devices featured.

Senior, John M. **Optical Fiber Communications: Principles and Practice.** 3rd edition, Prentice Hall, 2009. 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. A good introduction to some of the devices featured.

Sze, S. M. and Kwok Kwok Ng. **Physics of Semiconductor Devices**. 3rd edition, John Wiley, 2007. 21 SZE/1A and 21 SZE/1B.

Wilson, J. and J. F. B. Hawkes. **Optoelectronics: An Introduction.** 3rd edition, Prentice Hall Europe, 1998. A good introduction to some of the devices featured.

Options Paper 1 Michaelmas Term

Dr M. Slota and Prof S.C. Speller

12 lectures

Magnetic & Superconducting Materials

Magnetic Materials (6 lectures)

- **Spins: a playground for quantum mechanics**
    - Quantum spin representations, tensors, operators, symmetry and density matrix;
    - Anisotropy and exchange: Stevens operators, exchange and super-exchange mechanisms, and the spin Hamiltonian;
    - Spin-lattice relaxation and coherence times
    - Measurement techniques. Static: VSM, torque SQUID magnetometers; dynamic: Recovery, Hahn echos, dynamic decoupling, MOKE, etc…
    - Applications: quantum information, drug labelling, micellar probes etc…
- **Nanoscale and molecular magnetism**
    - Superparamagnetism: static and dynamic response
    - Different types of nanomagnets (oxides, metals, molecular etc…) and their fabrication: top down and bottom up approaches,
    - One-dimensional systems: Heisenberg and Ising chains, spin waves,
    - Applications: biology and medicine, magnetic storage, etc…
- **Spintronics**
    - Basic principles, operating mechanisms and outstanding questions
    - Magnetic tunnel junctions and spin valves;
    - Quantum behaviour of devices at the Nanoscale;
    - Molecular Spintronics
    - Applications: read heads, MRAM, racetrack memory, neuromorphic logic, single-spin sensors,

Superconducting Materials (6 lectures)

- **Fundamentals of superconductivity (quick recap from 2nd year)**
    - Critical parameters
    - Thermodynamics of the superconducting transition
    - London equation
    - Macroscopic quantum coherence and Cooper pairs
    - Type I and type II superconductivity
- **Properties of type II superconductors**
    - Flux lines
    - Flux pinning and critical currents
    - Reversible and irreversible behaviour
    - The Bean model
- **Tailoring microstructure in low temperature superconductors for magnet applications**
    - NbTi wires
    - Guest lecture on MRI (Siemens Healthineers) tbc
    - Nb_3Sn wires
- **Superconducting thin films for device applications**
    - The Josephson Effect
    - Fabrication of Josephson Junction devices
    - Superconducting Quantum Interference Devices (SQUIDS)
    - Passive microwave devices
- **High temperature superconductors (HTS) and applications**
    - Cuprate compounds
    - Grain boundaries in HTS
    - Bi-2212 wires
    - REBCO coated conductors
    - Guest lecture on HTS for fusion (Greg Brittles, Tokamak Energy) tbc
    - REBCO bulks for levitation and compact magnets
- **Novel superconducting materials**
    - Discovery of new superconductors
    - Magnesium diboride
    - Iron-based compounds
    - Room temperature superconductors – the hydrides

Further reading

Annett, James F. **Superconductivity, Superfluids, and Condensates**. Oxford University Press, 2004. Oxford Master Series in Condensed Matter Physics. Excellent book but more advanced than needed for this course.

Blundell, Stephen. **Magnetism in Condensed Matter**. Oxford University Press, 2001. Oxford Master Series in Condensed Matter Physics. Online.

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

Evetts, J. et al. **Concise Encyclopedia of Magnetic & Superconducting Materials.** Pergamon, 1992. Advances in Materials Science and Engineering. Dept. of Materials Library 21 EVE. Good reference book on a wide range of superconducting materials and applications.

Gatteschi, D. et al. **Molecular Nanomagnets**. Oxford University Press, 2006. Oxford Scholarship Online.

Girvin, Steven M. and Kun Yang. **Modern Condensed Matter Physics**. Cambridge University Press, 2019.

Griffith, J. S. **The Theory of Transition-Metal Ions**. Cambridge University Press, 2009.

Kittel, Charles and Paul McEuen**. Introduction to Solid State Physics**. Global edition, Wiley, 2018.

Maekawa, S. **Concepts in Spin Electronics**. Oxford University Press, 2006. Oxford Scholarship Online.

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.

Nazarov, Yuli V. and Yaroslav M. Blanter. **Quantum Transport: Introduction to Nanoscience**. Cambridge University Press, 2009. Cambridge Core.

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

Speller, Susannah. **A Materials Science Guide to Superconductors: And How to Make Them Super**. Oxford University Press, 2022. Superconductors. 21 SPE.

Options Paper 1 Michaelmas Term

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

12 lectures

Microstructural Control in Engineering Alloys

Aluminium Alloys (3 lectures)

- Aluminium Alloys: Recap Key series 2000, 5000, 7000 and aluminium silicon casting alloys; Al-Li and Al-Scandium alloys - Properties, processing, opportunities.

Steels (4 lectures)

- FeC recap – beyond alpha gamma phase transformations
- Martensitic steels: modern approaches to understanding martensitic formation; TRIP/TWIP
- Bainitic Steels
- HLSA Steels: thermomechanical treatments to control carbides
- FeCrNi alloys: spinodal decomposition and corrosion protection; precipitation strengthened Stainless steels for higher strengths.

Titanium Alloys (2 lectures)

- Alpha/beta alloys: processing for use in aerospace industry.
- Near Alpha alloys: alloy design for high temp
- Oxidation resistance of titanium
- Beta – alloy design for trade-off between strength and fracture toughness
- Intermetallics: TiAl system as used in GENX engine; processing routes, Order-disorder reactions

Magnesium Alloys (2 lectures)

- Cast Alloys, Wrought Alloys, Future opportunities

Nickel Super Alloys (1 lecture)

- What they are: alloy additions
- Nucleation and growth and coarsening of gamma prime
- Anomalous yield (revision), single crystal vs poly crystal

Essential reading

Bhadeshia, H. K. D. H. and R. W. K. Honeycombe. **Steels: Microstructure and Properties.** Fourth edition edition, Butterworth-Heinemann, 2017. Fundamental book for steel processing.

Leyens, C. and M. Peters. **Titanium and Titanium Alloys: Fundamentals and Applications**. Wiley-VCH, 2003. Dept. of Materials Library 52 LEY. Fundamental book for Titanium alloys.

Further reading

Campbell, John. **Complete Casting Handbook: Metal Casting Processes, Metallurgy, Techniques and Design.** Second edition, Elsevier: Butterworth-Heinemann, 2015. Chapter 6 -casting alloys,

Llewellyn, David T. **Steels: Metallurgy and Applications**. 2nd edition, Butterworth-Heinemann, 1994. Dept. of Materials Library 51 LLE/C. Chapters 'Engineering steels' and 'Stainless steels'

Rollett, Anthony et al**. Recrystallization and Related Annealing Phenomena**. London: Elsevier, 2017. Solid-state transformation fundamentals

Options Paper 2

Options Paper 2 Hilary Term

Prof D.E.J. Armstrong, Prof S. Lozano-Perez and Prof T.J. Marrow

12 lectures

Materials for Nuclear Systems

Introduction to Nuclear systems (3 lectures)

- What is nuclear fission, how do we extract energy from it?; Elastic Scattering and Inelastic scattering, neutron capture and activation, fission process, neutron cross-section, nuclear fuel cycle
- Reactor designs Gen III(+) and selected (IV); Key reactor components: fuels, cladding, moderators, cooling systems, pressure vessels, safety systems,
- What is Nuclear fusion and can we extract energy from it?; Fusion principles, reactor design, plasma containment, first wall materials, divertors, tritium production, latest developments.

Radiation damage and radiation induced microstructural evolution (4 lectures)

- Irradiation damage: Knock-on atoms and displacement cascades; Kinchen-Pease Model; Modifications to KP; Irradiation induced Dislocation loops; Nucleation of cavities and voids
- Radiation enhanced diffusion, Radiation induced segregation, Precipitate growth, Grain boundary segregation, Damage sinks
- Differences in irradiation damage between ions and neutrons
- Effects of irradiation damage on properties (selected examples)

Material Aging in Nuclear Systems (5 lectures)

- Thermal aging of reactor steels and microstructural evolution in RPVS (late blooming phases)
- Aging of graphite
- Hydride formation in Zirconium alloys
- Oxidation of zirconium alloys in LWRs
- Stress corrosion cracking and irradiation-assisted stress corrosion cracking

Further reading

Andresen, Peter L. and Gary S. Was. "**A Historical Perspective on Understanding Iascc**." Journal of nuclear materials, vol. 517, 2019, pp. 380-392.

Charit, Inajit and K. Linga Murty. **An Introduction to Nuclear Materials: Fundamentals and Applications.** Wiley-VCH, 2013.

Gorman, J.A. **"2015 Frank Newman Speller Award: Stress Corrosion Cracking and Nuclear Power**”. Corrosion, 2015, 71, 12, pp.1414. Available in RSL

Lozano-Perez, Sergio et al. "**SCC in PWRs: Learning from a Bottom-up Approach**." Metallurgical and materials transactions. E, Materials for energy systems, vol. 1, no. 2, 2014, pp. 194-210.

Marsden, B. J. et al. "**Dimensional Change, Irradiation Creep and Thermal/Mechanical Property Changes in Nuclear Graphite.**" International materials reviews, vol. 61, no. 3, 2016, pp. 155-182.

Motta, Arthur T. et al. **Hydrogen in Zirconium Alloys: A Review.** Journal of nuclear materials, vol. 518, 2019, pp. 440-460.

Motta, Arthur T. et al. **Corrosion of Zirconium Alloys Used for Nuclear Fuel Cladding.** Annual review of materials research, vol. 45, no. 1, 2015, pp. 311-343.

Murray, Raymond L. and Keith E. Holbert. **Nuclear Energy: An Introduction to the Concepts, Systems, and Applications of Nuclear Processes**. Eighth edition, Butterworth-Heinemann, 2020.

Murty, K. L. and I. Charit. **Structural Materials for Gen-Iv Nuclear Reactors: Challenges and Opportunities**. Journal of nuclear materials, vol. 383, no. 1, 2008, pp. 189-195.

Odette, G. R. et al. **On the History and Status of Reactor Pressure Vessel Steel Ductile to Brittle Transition Temperature Shift Prediction Models**. Journal of nuclear materials, vol. 526, 2019, p. 151863.

Scott, Peter M. and Pierre Combrade. **General Corrosion and Stress Corrosion Cracking of Alloy 600 in Light Water Reactor Primary Coolants**. Journal of nuclear materials, vol. 524, 2019, pp. 340-375.

Soneda, Naoki. **Irradiation Embrittlement of Reactor Pressure Vessels (Rpvs) in Nuclear Power Plants**. 1st edition, Woodhead Publishing, 2014.

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.

Was, Gary S. **Fundamentals of Radiation Materials Science: Metals and Alloys**. Second edition, Springer, 2016.

Was, G. S. et al. **Materials for Future Nuclear Energy Systems**. Journal of nuclear materials, vol. 527, 2019, p. 151837.

Options Paper 2 Hilary Term

Prof H. Bhaskaran

12 lectures

Enabling Nanotechnology - From Materials To Devices

Nanotechnology in Devices (6 lectures)

- Device scaling to the nanoscale and integrated circuits (4)
- Solid-state Memory and novel in-memory computing (Distinguished Industry Guest Lecturer, Dr Abu Sebastian) (1)
- MEMS and NEMS (1)

Nanofabrication (3 Lectures)

- Lithography, Etching and Deposition, Doping and activation, Novel patterning approaches

Nanoscale Materials and Characterization (3 Lectures)

- Nanoscale film deposition techniques overview, Emerging Nanoscale Materials, Challenges in characterization and overview of techniques (2)
- Scanning Probe Microscopies and other emerging techniques (Distinguished Industry Guest Lecturer, Dr Bernd Gotsmann)

Further Reading

Hornyak, Gabor L. **Introduction to Nanoscience**. CRC ; Taylor & Francis [distributor], 2008. Dept. of Materials Library 58 HOR/2. 58 HOR/2.

---. **Introduction to Nanoscience & Nanotechnology**. CRC ; Taylor & Francis [distributor], 2009. Introduction to Nanoscience and Nanotechnology. 58 HOR.

Madou, Marc J. **Fundamentals of Microfabrication and Nanotechnology**. Third edition, CRC Press, 2011. Solid-State Physics, Fluidics, and Analytical Techniques in Micro- and Nanotechnology.

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.

Further 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. This 3rd revised edition specified.

---. **Biological Performance of Materials : Fundamentals of Biocompatibility**. 4th edition, Taylor & Francis, 2006. online. 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. 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. This edition specified.

Park, Joon Bu. **Biomaterials Science and Engineering.** Plenum, 1984. Dept of Materials Library 45 PAR.

Ratner, B. D. et al. **Biomaterials Science : An Introduction to Materials in Medicine**. Third edition, Elsevier: Academic Press, 2013. Online. This 3rd edition specified.

Vaughan, Janet. **The Physiology of Bone**. Third edition, Clarendon Press, 1981. Oxford Science Publications. Online. 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.

Options Paper 2 Hilary Term

Dr M. Forghani

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:

- 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
- Crystallization
- Interface phenomena
    - Polymer miscibility
- 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

Neutron scattering as a tool for the study of polymeric materials

- Neutron vs. X-ray vs. Light Scattering
- Scattering concepts and fundamentals of neutron scattering:
    - Elastic and Inelastic Scattering
    - Momentum Transfer, Q
    - Scattering Cross Sections

        - Length scales
- Quasi-Elastic Neutron Scattering (QENS): The study of polymer dynamics
    - Coherent and Incoherent Scattering
    - Transmission
    - Linewidth analysis and geometry
- Small Angle Neutron Scattering (SANS): The study of polymer structure
    - Contrast matching
    - The single particle (shape) factor, P(Q)
    - The inter-particle structure factor, S(Q)
    - Analysis via standard plots
- Polymer samples and examples
    - Polymer blends
    - Polymer films
    - Reflectivity techniques
    - Capillary waves

Essential 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. 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. Chapters 3, 5, 8 & 12.

Further reading

Ashby, M. F. **Materials and the Environment: Eco-Informed Material Choice**. Third edition, Butterworth-Heinemann, 2021. 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. For lectures 9-12 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. Chapters 2 & 5.

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. 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. Chapter 13.

Olabisi, Olagoke et al. **Polymer-Polymer Miscibility.** Academic Press, 1979.

Pethrick, R. A. and J. V. Dawkins. **Modern Techniques for Polymer Characterisation.** Wiley, 1999. For lectures 9-12 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 9-12 on Neutron Methods and Recycling issues

Young, Robert J. and Robert Nobbs Haward. **The Physics of Glassy Polymers**. 2nd ed edition, Chapman & Hall, 1997. Chapters 9 & 10.

Options Paper 2 Hilary Term

Prof J.M. Smith

12 lectures

Quantum Technology

This course will introduce quantum technologies and the key materials used in their development and realization. It will begin with an introduction to the concepts grounded in elementary quantum physics, and will then address each of the three application areas of quantum technology, namely sensing, communications and computing. For each application area the principal approaches and materials used will be discussed, along with some of the outstanding materials challenges in realizing the full potential of quantum technology to bring about the “third industrial revolution”.

1. Basic Concepts (3 lectures)

- What is quantum technology?
- Qubits and measurement
- Entanglement and quantum logic
- Decoherence

2. Quantum Sensing (2 lectures)

- Single photon detection
- Field sensing using quantum devices

3. Quantum communications (2 lectures)

- Single photon sources
- Entangled photon sources
- Quantum memories and the quantum internet

4. Quantum simulation and computing (5 lectures)

- Superconducting circuits
- Trapped ions and cold atoms
- Photons
- Semiconductor quantum dots
- Colour centres in wide gap materials
- Quantum simulation of materials

Further Reading

Bouwmeester, Dirk et al. **The Physics of Quantum Information: Quantum Cryptography, Quantum Teleportation, Quantum Computation**. Springer, 2000. Dept. of Materials Library 20 BOU.

Doherty, Marcus W. et al. "**Quantum Science and Technology Based on Color Centers with Accessible Spin**." Journal of Applied Physics, vol. 131, no. 1, 2022, p. 10401, doi:10.1063/5.0082219.

Fox, Mark. **Quantum Optics: An Introduction.** Oxford University Press, 2006. Oxford Master Series in Physics; 15. Includes bibliographical references (p. [360]-368) and index.

Oliver, William D. and Paul B. Welander. "**Materials in Superconducting Quantum Bits**." MRS Bull, vol. 38, no. 10, 2013, pp. 816-825, doi:10.1557/mrs.2013.229.

Articles in Materials for Quantum Technology, the new journal by Institute of Physics Publishing: https://iopscience.iop.org/journal/2633-4356

Options Paper 2 Hilary Term

Prof M.S. Islam, Prof M. Pasta and Prof R.S. Weatherup

12 lectures

Energy Materials

Li-ion batteries and beyond (4 lectures)

Lecture 1: Introduction

- Importance of batteries
- Electrochemical thermodynamics: energy density
- Electrochemical kinetics: power density
- Lithium-ion batteries: basic structure and nomenclature
- Beyond lithium-ion

Lecture 2: Cathodes

- Li-ion cathodes: state of the art (LCO, NMC, LFP)
- Li-ion cathodes: forefront (O-redox, sulphur, oxygen, metal fluorides)
- Beyond lithium-ion cathodes

Lecture 3: Anodes

- Li-ion anodes: state of the art (graphite)
- Li-ion anodes: forefront (silicon and lithium)
- Beyond lithium-ion anodes

Lecture 4: Electrolytes

- State of the art: liquid electrolytes
- Novel electrolytes: solid-state electrolytes

Hydrogen and sustainable fuels (4 lectures)

Lecture 1: Introduction, thermodynamics, and kinetics of catalysis

- The hydrogen society
- Critical role of catalysis
- Catalysis basics

Lecture 2: Thermocatalysis

- Alternative fuels produced from hydrogen
- Le Chatelier's principle

- Fischer-Tropsch, methanol, and ammonia synthesis
- Hydrogen generation from fuels

Lecture 3: Electrocatalysis)

- Structure and operation of solid oxide and polymer electrolysers/fuel cells
- Electrocatalyst selection for HER/OER
- Measuring electrocatalyst performance
- Origin of potentials at the electrode/electrolyte interface

Lecture 4: Realising TW-Scale Hydrogen Production

- Demand for hydrogen
- State of current technology
- Resource availability
- Outstanding materials challenges

Solar (4 lectures)

Lecture 1: Principles of solar energy conversion

- History of solar cells
- Thermodynamic treatment of PV operation
- Semiconductor treatment of PV operation
- Cell architectures
- Losses and efficiency limits

Lecture 2: Mainstream crystalline silicon solar cells

- Design and production of silicon solar cells
- Defect engineering in silicon
- Thin film interface materials on silicon
- Metallisation technology
- Impact of defects in practical PV devices

Lecture 3: Perovskite materials for solar cells

- Perovskite structure and materials
- Optoelectronic properties
- Defect and transport properties
- 2D perovskite materials

Lecture 4: Perovskite solar cell devices

- Solar cell architectures
- Solar cell parameters and characterisation
- Interface properties
- Tandem perovskite-silicon cells

Further Reading

Huggins, Robert A. **Advanced batteries: materials science aspects.** Springer (2009).

Fuller, Thomas Francis et al. **Electrochemical engineering.** Wiley (2018). [Chapters 1-8]

Chorkendorff, I. **Concepts of modern catalysis and kinetics.** Wiley (2017) [Chapters 1, 2, 3, 6, 8]

Nelson, Jenny. **The physics of solar cells.** Imperial College Press (2003) [Chapters 1,2,4 and 7]

Grätzel, Michael et al. **Perovskite solar cells: materials, processes, and devices.** Wiley (2021).

Fujiwara, Hiroyuki. **Hybrid perovskite solar cells: characteristics and operation.** Wiley (2022).

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 1 and 2 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 7th week of Michaelmas Term. There will be a pre-sign up meeting in week 5 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. R.J. Nicholls and Dr E. Demir

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

Further reading

Allen, M. P. and D. J. Tildesley. **Computer Simulation of Liquids.** Clarendon Press, 1989. Dept. of Materials Library 12 ALL. Both editions ok.

Dunne, Fionn and Nik Petrinic. **Introduction to Computational Plasticity.** Oxford University Press, 2005. Ebook Central.

Frenkel, Daan and Berend Smit. **Understanding Molecular Simulation: From Algorithms to Applications.** 2nd edition, Elsevier Science, 2001. Computational Science Series.

Giustino, Feliciano. **Materials Modelling Using Density Functional Theory: Properties and Predictions.** Oxford University Press, 2014. Dept. of Materials Library 10 GIU.

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

Options Module Weeks 1 & 2, Hilary Term

Prof. M.P. Moody, Prof. M.L. Galano and 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 materials characterization techniques. The remaining period will be devoted to training, 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 30 marks. The reports will be submitted by midday Tuesday of week 3, Hilary Term. A model report will be available to provide some guidance.

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:

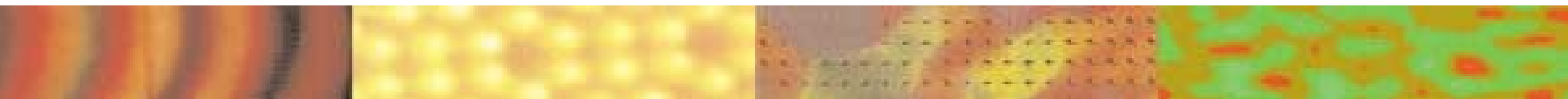
Each student will write a project report (max. 3000 words) describing their computational characterisation, which will be marked by the assessors out of a maximum of 30 marks. The projects will be assigned at the end of the first week to be completed autonomously during the second week, with reports due in by midday Tuesday of week 3, Hilary Term.

Further reading

Giustino, Feliciano. **Materials Modelling Using Density Functional Theory: Properties and Predictions.** Oxford University Press, 2014. Dept. of Materials Library 10 GIU.

Hafner, Jürgen. **"Ab-Initio Simulations of Materials Using Vasp: Density-Functional Theory and Beyond."** Journal of Computational Chemistry, vol. 29, no. 13, 2008, pp. 2044-2078, https://doi.org/10.1002/jcc.21057

Hasnip, Pj et al. **"Density Functional Theory in the Solid State."** Philos. Trans. R. Soc. A-Math. Phys. Eng. Sci., vol. 372, no. 2011, 2014. https://doi.org/10.1098/rsta.2013.0270
Kohanoff, Jorge. **Electronic Structure Calculations for Solids and Molecules: Theory and Computational Methods.** Cambridge University Press, 2006.
Martin, Richard M. **Electronic Structure: Basic Theory and Practical Methods.** Cambridge University Press, 2004. Cambridge Core.



Department of Materials
University of Oxford
Parks Road
Oxford OX1 3PH
United Kingdom

Tel +44 (0)1865 273700
Fax +44 (0)1865 273789
Email enquiries@materials.ox.ac.uk
Web www.materials.ox.ac.uk