

Postgraduate Lecture & Training Course Synopses
2024-25
and Research Colloquia Details

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Postgraduate Lecture & Training Course Synopses and Research Colloquia Details 2024-25

This booklet contains the synopses of postgraduate courses in the Department of Materials for 2024-25. **'Postgraduate training'** courses provide essential training for using some of our research facilities and a selection of transferable 'career skills' training (which is a requirement of many sponsors of research degrees). If you are a probationer research student, in addition to the compulsory safety lecture you are required to attend the workshops and lectures listed under **mandatory skills training**. **'Postgraduate teaching'** courses are intended to broaden and deepen your education by offering you more advanced material both in areas within and outside your own research. This booklet also contains synopses of the undergraduate **third year materials options** from our MEng degree programme. Synopses of lecture courses offered to first and second year undergraduates are contained in separate booklets.

Postgraduate training courses offered by the Mathematical, Physical and Life Sciences Division can be viewed via the [MPLS Graduate School](#) webpages. Information on lecture courses offered by other departments of the MPLS Division and the University normally can be found via department webpages and at [Lecture Lists](#) .

If you are a probationer research student you will be required to offer two subjects during the first year for assessment. One of these subjects must be in an area outside your research topic. You should first consult your supervisor and, if necessary, the Director of Graduate Studies (Dr Adrian Taylor) about the selection of your two topics for assessment. Your selection may be made from any of the courses listed under **Postgraduate teaching**, or the **third year options** (provided you have not already taken the option as an undergraduate), or other **postgraduate lecture courses available within the Mathematical, Physical and Life Sciences Division**.

It is essential that your performances on the two courses you select are assessed. To pass an assessed course you must (i) normally have attended a significant proportion of the complete course of lectures (some lecturers will define this more specifically in the synopsis for the course) and (ii) obtain a grade of at least 50% on the written work set by the lecturer (this is equivalent to a 'pass' at MSc level and is regarded as satisfactory for the purpose of transfer of status.)

- SOME OF THE LECTURE COURSES COMMENCE EARLY IN MICHAELMAS TERM, SO PLEASE CONSULT YOUR SUPERVISOR PRIOR TO THIS.
- IF YOU ARE UNDERTAKING AN ELECTRON MICROSCOPY (EM) TRAINING MODULE YOU MAY NEED TO TAKE A PARTICULAR POSTGRADUATE LECTURE COURSE. IN SUCH CASES YOUR SUPERVISOR SHOULD HAVE LIAISED WITH THE EM SUPPORT STAFF BEFORE YOUR PROJECT COMMENCED AND WILL BE ABLE TO ADVISE YOU ON THIS. THE EM SUPPORT STAFF WILL PROVIDE YOU WITH A SCHEDULE FOR YOUR EM TRAINING. PLEASE SEE [P33](#) FOR INFORMATION ON ARRANGING EM MODULAR TRAINING.

The Department's formal research colloquium series is normally held on selected Thursdays throughout term at 4.00 pm in the Hume-Rothery lecture theatre. If you are a probationer research student you will be required to attend a minimum of seven colloquia during Michaelmas and Hilary terms of your first year, to include at least three of these Departmental Colloquia. Evidence of this attendance will be required, as described in the Graduate Student Handbook. See section 9 of the Materials Graduate Student Handbook for guidance if you wish to offer towards this course requirement colloquia you have attended in another Department or Materials colloquia other than our Thursday afternoon series. You should check www.materials.ox.ac.uk for the final version of the list of colloquia. Information about colloquia in Hilary and Trinity terms will be distributed later in the academic year, and posted on the web site. Everyone in the Department with an interest in research is encouraged to attend the colloquia and hear of cutting-edge research across a broad range of the science and engineering of materials. The colloquia also provide a means to interact with other members of the Department and the speaker during tea before or after the talk.

Dr Adrian Taylor
Director of Graduate Studies

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Postgraduate Training Mandatory

Postgraduate Training: Mandatory

Michaelmas Term

Organised by Dr A.O. Taylor

1 session of 2-3 hours led by Dr Paul Warren, ex NSG (Pilkington Glass), assisted by Dr Adrian Taylor

Project Management

This two to three hour course introduces the application of basic project management to the research undertaken for a research degree. It will cover topics such as defining a DPhil project, structuring the research and associated activities and managing their progress. The aim is to teach new research students techniques which will help them to complete successfully their degree within the funded period for the degree. Experience of project management is also a useful generic skill and one that is valued by graduate recruiters

The Department's graduate course structure includes six-monthly project management reviews. This allows and encourages you as the student to take responsibility for the successful outcome of your research by assessing expectations and progress throughout the duration of your course. It will enable you to flag up any concerns you might have that your research is not keeping to schedule, so that your supervisor and, if necessary, the Materials Graduate Studies Committee can consider whether remedial action is required.

You are expected to bring a first draft of your Project Management Form 1 (excluding the Gantt Chart and WBS) to the afternoon seminar of the workshop.

Postgraduate Training: Mandatory

Michaelmas Term

Dr A.O. Taylor

(A Careers Advisor from the OU Careers Service)

1 session of 1.5 hours

Looking to the Future – What do employers seek?

A guide to the qualities and skills sought by employers; given in year one to enable you to deliberately develop these qualities, thus maximising your chance of winning your 'dream job' in due course. Careers in industry and academia are covered.

tbc

1 hour

Safety Lecture

A guide to the Departmental Safety Policy as described in the Safety Organisation and Laboratory Safety documents. Provides an outline from the Departmental Safety Officer about how risks are formally assessed, what to do in an emergency, how to access help and report incidents, training and first aid. Also identifies sources of relevant information.

Compulsory for all new research workers

Postgraduate Training

Where a synopsis is shown in grey font, the course or workshop will not be offered in 2024/25 but may be offered in subsequent years

Postgraduate Training

Michaelmas Term

Dr S. Boad (Institute of Materials, Minerals & Mining)

1 session of 1 hour

The Institute of Materials, Minerals & Mining (IoM³)

An introduction to the professional body for Materials Scientists. For those first year research students who attend this talk and do not already have student membership of the Institute the Department will pay for your student membership of the IoM³ for your first year.

Postgraduate Training
Radcliffe Science Library
1 session of 1h 30mins

Michaelmas Term

Information Skills

This session will introduce you to the electronic sources of scientific information used by Materials Scientists and how to access and search them, focussing on:

- Use of SOLO for searching Oxford Library Collections
- Electronic resources for Materials Science research
- General principles for a comprehensive literature search
- Effective use of electronic databases Materials Research Database, Web of Science and SciFinder (chemistry) as examples
- Finding e-journals and conference proceedings
- Citation searching using the Web of Science
- Copyright and plagiarism (introduction)

There will be hands-on practice and an opportunity for students to discuss their projects.

(Use of the standard search engines for the World Wide Web will not be covered in any detail, as these will be familiar to most people. However there are additional lectures organised by the University Computing Service if you feel you need some help in this area.)

Postgraduate Training
Radcliffe Science Library
1 session of 2 hours

Hilary Term

Managing your References (Bibliographic Software)

This 2-hour session will introduce you to software tools used to organise your references. Reference Management software such as EndNote and RefWorks will be demonstrated to help you export references as you search databases, library catalogues and the Internet, and create bibliographies when you require them.

Further options of using 'Write as you cite' software to add in-text citations and create a Reference List using appropriate referencing style will also be shown. Practical part of the session includes exploring 'RefWorks' software for collecting, organising and managing your references.

Additional session on managing your references is organised as part of the WISER Program. This session provides a comparison of five software tools to help you choose the software that suit your needs.

Postgraduate Training
Radcliffe Science Library
1 session of 2 hours

Michaelmas Term

Patent Literature

This session provides an introduction to patent literature, to where patents can be found and how to search patent databases and obtain full-text patent information.

Searching for patent information will also be demonstrated in materials science and chemistry research databases using the Proquest platform and SciFinder database. Further examples include tracking patent application, or finding a specific patent in databases.

The session will include hands-on searching of patent databases.

This session does not cover any legal issues related to use of patents.

Postgraduate Training

Dr A.O. Taylor

Poster Presentation Skills

Dr Taylor's slides from a workshop that is no longer offered are available at Postgraduate Skills Training

Posters are widely used at scientific conferences and in this workshop guidance will be given on how to make effective use of this medium.

During Hilary term a Departmental DPhil Poster session will be held to give practical experience (Year 3 students will present posters). Two prizes, each of £200, are sponsored:

1. Best "Scientific Conference" entry (sponsored by Rolls-Royce).
2. Best "Public Understanding" entry (sponsored by the Ironmongers Company).

Postgraduate Training

Michaelmas Term

Dr Abby Evans (OU Careers Service)

1 session of 1 hour

The OU Careers Service – Active Job Hunting

An introduction to the support available from OUCaS to students and post-docs reaching the end of their research and who are seeking jobs.

Postgraduate Training

Michaelmas Term

Dr A.O. Taylor and others, including several alumni

1 session of approximately 2 hours

Careers and Networking Event with Alumni

An opportunity for informal discussion of careers available to Materials graduates, with several alumni of the Department representing a broad range of employment sectors.

Informal one-to-one chats are held over a glass of wine or soft drink in the Holder Café.

Biographies of those alumni who are participating will be provided in advance.

This event will be useful both (i) if you already know in which sector you would like to work, in which case you can seek “insider” knowledge from specific alumni or (ii) if you are simply seeking inspiration for the direction in which your Materials degree might now take you.

Presentation Skills

What is it that makes a good talk? As scientists, we constantly need to convey information about our work and explain new results, so it is important for us to have good presentation skills. Most scientific and other presentations are given using electronic media, especially using software such as PowerPoint. This is just a method of presentation, and while it allows a wider range of techniques, computer presentation is no more a guarantee of a good talk than the use of a blackboard is proof of a bad one. These sessions will aim to give some insight into how you should prepare, structure and present your talks in order to get your message across. Hints will also be given as to how to use computer presentation methods effectively, based on PowerPoint, which is available through a University site license. The course will comprise four sessions:

- PowerPoint for scientific presentations, including hands-on practice (ITS Level 3 course; basic knowledge of PowerPoint is assumed).
- An introduction to advanced audio-visual technology (including Touch Screens and Visualisers).
- Production of posters using PowerPoint.
- Practical tips on delivering a research talk.

It is permissible to attend just those sessions in which you are interested.

Postgraduate Training

Hilary Term

OU Language Centre

5 sessions of 2 hours

10 places only

Academic Writing (for overseas students)

This intensive course runs over five consecutive afternoons and is aimed at students for whom English is a second language, with priority given to those who are finding it difficult to write reports in English. If you have already attended one of the Language Centre's courses on Academic Writing please contact Sharmaine Ijada (graduate.studies@materials.ox.ac.uk) to determine if the present course will be of any value to you.

Postgraduate Training

All Terms

Dr E. Liotti

Each visit requires approx 4 hours (including travel time)

Industrial Visits

If places are available, research students may join one or more of the several visits that are arranged each year to industrial sites to illustrate some of the applications of Materials Science.

Industrial Tour

Some places may be available on the Industrial Tour. A visit of 5-10 days, usually during the Easter Vacation, is made to a region overseas in order to visit several companies that make use of Materials Science. Recent visits were to California, Poland, Sweden, China, the south of France, Singapore, and Germany.

Several talks, each typically 40-60 minutes

Industrial Talks

Each year, scientists from Rolls Royce, Tata Steel and Johnson Matthey visit the Department to give short talks on the applications of Materials Science in industry. Often these talks are followed by a buffet lunch during which you can network with the industrialists and learn of career opportunities.

In addition the Department's very active Student Materials Society ('MatSoc') normally arranges several events each year including some talks given by external speakers (have a look at <https://www.matsoc.com/events>). Hence you might wish to consider joining MatSoc.

Owning a Successful DPhil

This is a 1 hour workshop organised and run by the student members of the JCCG. It is very much 'by students for students', and covers some inside advice about the following topics:

Motivation;

Working Hours;

Deadlines & Finishing On-time;

Expectations –

 “What does my supervisor expect from me?”

 “What do you want from your supervisor?”

The truth about doing a DPhil;

Organising a long project;

Internal & External Resources.

The workshop is followed by lunch over which you will have the opportunity to talk with older DPhil students (3rd/4th years) and some post-docs about their experiences.

Teaching Skills

A series of workshops to introduce the topic to those new to teaching and to enable existing teachers to share experiences & best practice.

- **Tutoring Maths Classes** Michaelmas Term
Prof S.C. Benjamin
3 hours
- **Tutoring Materials Science** Michaelmas Term
tbc
3 hours
- **Materials Options Classes** Michaelmas Term
Prof M.L. Galano
3 hours (2h if delivered virtually by MS Teams)
[Please note: This workshop is run only if required]
- **Junior Demonstrating in the Materials Teaching Lab** Michaelmas Term
Prof D.E.J. Armstrong and D.R. Passmore
1.5 hours
In addition to the workshop, one-to-one mentoring is provided by the Senior Demonstrator(s) for the experiment(s) you are “demonstrating”, and you are required to practise the full experiment in advance of the actual lab classes.
- **Senior Demonstrating**
One-to-one mentoring is provided by the Practical Courses Organiser (Prof D.E.J. Armstrong) and normally a Senior Demonstrators’ forum is arranged once or twice each year for the sharing of best practice, etc.

- **Lecturing a Taught Course**

Prof T.J. Marrow

3 hours

[Please note: This workshop is run only if needed.]

This workshop is aimed particularly at those who might have to deliver all or part of an **existing** lecture course to undergraduates or taught MSc students, for example if covering for a member of staff on sabbatical leave. It is also open to others who are interested and keen to develop this area of their CV.

The workshop will include:

- The expectations of colleagues and students.
- The lecture in its context as one part of an integrated 'unit of study' (e.g. an Oxford 'Paper' or, elsewhere, a 'Module').
- A digest of the relevant educational research on student learning by means of lectures.
- Practical tips on delivering a lecture course.
- Open discussion to share opinions on 'best' practice.

[Note: the workshop will **not** cover topics such as writing a **new** lecture course, syllabus design or delivering a research talk; these topics either are or will be covered in other workshops].

See also Teaching Skills workshops run by the MPLS Division, advertised at

<https://www.mpls.ox.ac.uk/training>.

Postgraduate Teaching

- **Graduate student teaching and training in electron microscopy**

User training takes place throughout the year in response to supervisors' EM access requests to support research projects. EM training is split into lectures on the theory behind techniques (see pages [34-39](#) of this document) and also practical training on the operation of instrumentation and collection of data.

Practical training builds upon the concepts covered in EM postgraduate lectures and is tailored to the applicants' specific research project. It is usually conducted in small groups or 1:1 and led by one of the EM Facility Research Support Scientists. Because training is tailored to match individual researchers' needs then there is no set syllabus. Topics include an introduction to practical operation of the scanning electron microscope, and similarly an introduction to the transmission electron microscope. EM facility staff may also offer practical training in further techniques such as energy dispersive X-ray analysis, electron energy loss spectroscopy, high-resolution EM, scanning transmission electron microscopy and specimen preparation as necessary for the progress of researchers' projects. All of these practical skills link in with the material covered in the EM-specific graduate lecture courses. Additionally support scientists provide instrument-specific practical training to teach users to safely and effectively operate instruments within the EM facility.

Some of our EM training is delivered through stand-alone modules covering advanced or specialist techniques dealing with aspects beyond the scope of the postgraduate lectures. These include topics such as focussed ion-beam milling, electron backscatter diffraction and advanced microanalysis. Full details are given in the 'Modular Courses in Electron Microscopy' section of the present synopses.

All EM related training can only be accessed through the EM access request process of the David Cockayne Centre for Electron Microscopy (DCCEM). Users are given a timetable for lectures/practical classes that they should attend at the start of their training. **In the case of a lecture course beginning early in MT, students should apply to emaccess@materials.ox.ac.uk to reserve a place. This is particularly important for the Foundation Topics for EM course as places are limited and prioritised for those who will make use of EM during their first year.** Further details are available in the departmental graduate handbook or at www-em.materials.ox.ac.uk/

Foundation Topics for Electron Microscopy

The course covers foundation level topics necessary for progress in both theoretical and practical understanding of electron microscopy (SEM, TEM & FIB). The syllabus concentrates on the basic physics of optical systems, waves, diffraction, the relation of these to the electron, plus properties of charged particles in E and B fields. Sample preparation and FIB are discussed in detail. Mathematical methods important to researchers using EM are also included and will be drawn upon in later postgraduate courses and training. All who wish to use SEM, TEM & FIB instrumentation within the department must attend the course and will be advised by EM support staff on the lectures most relevant to them. The course may also be taken for credit, see below.

Lecture 1: Optics: Basics, refractive index, Snell's law, dispersion, properties of thin lenses, magnification. The optical microscope, comparison to electron microscopy.

Lecture 2: Quantum physics of electrons and practical EM: Wave interference, diffraction. Quantum nature of the electron and relation to EM. Magnetic fields, simple magnetic lenses, electric field, actions on charged particles.

Lecture 3: The vacuum: Concept, gases, gas-laws, measurement, chambers, pumps, outgassing, partial pressures, vapour pressure, contamination.

Lecture 4: Specimen preparation for EM: Scientific considerations for SEM and TEM. Overview of preparation techniques and suitability to various materials and applications.

Lecture 5: Focused ion beams: Introduction to FIB and LMIS, milling and imaging with ions, deposition, applications

Lecture 6: FIB-SEM Instruments: The FIB-SEM concept, field emission SEM, imaging and contrast, example applications. Pros and cons of FIB-SEM

Lecture 7: Mathematical topics for EM I: Discrete sampling, aliasing, Poisson distribution. Nyquist Frequency. Waves, Fourier Transforms, Spatial frequencies, application in EM.

Lecture 8: Mathematical topics for EM III: Convolutions, cross correlations, links to EM, image processing, image filtering.

Pre-requisites: None

Postgraduate Assessment:

Students will be assessed at the end of the course on their written answers to several questions. In addition, students can only be assessed if they have attended a minimum of six lectures.

Further Reading

Williams, D. B., & Carter, C. B., **Transmission Electron Microscopy**, Plenum

Reimer, L., **Transmission Electron Microscopy**, Springer-Verlag

Pennycook, S.J. & Nellist, P.D., **Scanning Transmission Electron Microscopy: Imaging and Analysis**, Springer

Bracewell, R., **The Fourier Transform & Its Applications**, McGraw-Hill

Microscopy and Analysis of Surfaces

This lecture course covers the main experimental techniques that are used to investigate the structure and composition of surfaces and the near surface region. In particular scanning electron microscopy, scanning probe microscopy, and surface chemical analysis techniques are discussed. The principles of operation are illustrated through numerous practical examples. Those wishing to use SEM instrumentation in their research must attend at least the three lectures on SEM.

Scanning Electron Microscopy (SEM) 1

Layout of the SEM, electron sources, electromagnetic lenses, secondary electron and back scattered electron detectors, image formation.

SEM 2

Electron - sample interactions in the SEM, elastic and inelastic scattering processes, interaction volumes, convolution of probe size and interaction volume, the signal to noise ratio and visibility criteria.

SEM 3

Advanced SEM imaging techniques, low voltage SEM, EBIC, EBSD, environmental SEM, voltage contrast, magnetic contrast, cathodoluminescence.

Scanning Tunnelling Microscopy (STM)

Principle of operation of the STM, atomic resolution imaging, atomic manipulation, electronic structure measurements with the STM.

Atomic Force Microscopy (AFM)

Principle of operation of the AFM, nanoscale imaging, related scanning probe microscopes (SPM).

Micro and nanomechanical techniques

Micro and nano-indentation, modifications to the AFM, force modulation microscopy and phase mapping.

Chemical analysis 1

Atom probe, secondary ion mass spectroscopy (SIMS). Raman spectroscopy, Photoluminescence.

Chemical analysis 2

Auger electron spectroscopy, X-ray photoelectron spectroscopy, EDX.

Postgraduate Assessment:

To obtain a pass credit for this course it is necessary to attend all the lectures (unless there are exceptional circumstances), and to provide satisfactory answers to the questions on the problem sheet.

Further Reading

Reimer, L., **Scanning Electron Microscopy: Physics of image formation & microanalysis**, Springer

Oatley, C. W., **The Scanning Electron Microscope**, Cambridge University Press

Thornton, P. R., **Scanning Electron Microscopy: Applications to materials and device science**, Chapman and Hall

Goodhew, P. J., & Humphreys, F. J., **Electron Microscopy and Analysis**, Taylor & Francis

Tsong, T. T., **Atom probe field-ion microscopy**, Cambridge University Press

Watts., F., **Introduction to Surface Analysis by Electron Spectroscopy**, Oxford Science Publications

Bonnell, D. A., **Scanning Probe Microscopy and Spectroscopy**, Wiley

Chen, C. J., **Introduction to Scanning Tunneling Microscopy**, Oxford University Press

Sarid, D., **Scanning Force Microscopy**, Oxford University Press

Wiesendanger, R., & Guntherodt, H-J., eds., **Scanning Tunnelling Microscopy II Further Applications and Related Scanning Techniques**, Springer-Verlag

Woodruff & Delchar, **Modern techniques of surface science**, Cambridge University Press

Spectroscopy with the (S)TEM

The lecture course describes spectroscopic modes which allow chemical analysis in the electron microscope. The content builds on that from the '[Foundation topics for electron microscopy](#)' course and centres on the two most widely employed techniques of Energy Dispersive X-ray (EDX) analysis and Electron Energy-Loss Spectroscopy (EELS). The course must be taken by those wishing to use EDX and/or EELS in their research. EM support staff will advise researchers on the lectures most relevant to them. The course may also be taken for credit, see below.

Lecture 1: X-rays: Generation, properties, production, structure of atom, selection rules, allowed and forbidden transitions, mean free path, ionisation cross-section.

Lecture 2: Detection of X-rays: Absorption coefficient, detector setup, charge pulse amplification, pulse processing, MCA, dead time, resolution, (instrument) artefacts.

Lecture 3: X-ray Spectrum Processing: Background removal, filtering, binary and multi-element specimens, standard vs standard-less analysis, detection efficiency, self absorption, detection limits.

Lecture 4: Other applications of X-rays: Real examples, Monte-Carlo modelling, ALCHEMI, Coherent Bremsstrahlung, STEM-EDX mapping, data cube.

Lecture 5: X-ray spectroscopy in SEM : Applications, differences from the transmission case, Wavelength dispersive spectroscopy (WDS), cathodoluminescence.

Lecture 6: EELS: Basics, inelastic scattering, phonons, ionisation process and notation. The EEL spectrum: zero loss, plasmons, core-loss, ELNES, EXELFS. Spectrometers. Example spectra.

Lecture 7: EELS II: Edge shapes, Quantification, simulation

Lecture 8: Advanced Analytical Techniques: Energy filtered TEM (EFTEM), chemical mapping, spectrum imaging, examples from research.

Pre-requisites: [Foundation topics for electron microscopy](#) lecture course.

Postgraduate Assessment:

Students will be assessed at the end of the course on their written answers to several questions. In addition, students can only be assessed if they have attended a minimum of six lectures.

Further Reading

Cowley, J. M., **Diffraction Physics**, North Holland

Reimer, L., **Transmission Electron Microscopy**, Springer-Verlag

Fitzgerald, A. G., et al., **Quantitative Microbeam Analysis**, SUSSP and IOP Publishing

Hren, J. J., et al., eds., **Introduction to Analytical Electron Microscopy**, Plenum

Egerton, R. F., **Electron Energy-Loss Spectroscopy in the Electron Microscope**, Plenum

Russ, J. C., **Fundamentals of Energy Dispersive X-Ray Analysis**, Butterworths

Reed, S. J. B., **Electron Microprobe Analysis**, Cambridge University Press

Flewitt, P. J., & Wild, R. K., **Physical Methods for Materials Characterisation**, IOP Publishing

Williams, D. B., & Carter, C. B., **Transmission Electron Microscopy**, Plenum

Imaging and Diffraction in (S)TEM

The lecture course covers the theory behind imaging and diffraction in TEM, explaining the origin of this data and how it may be interpreted. High-resolution phase contrast TEM (HRTEM) is discussed, in addition to Scanning Transmission Electron Microscopy (STEM) imaging. A brief overview of electron-optical aberration-correction is included with reference to the topics of HRTEM and STEM. The course builds upon the material covered in the '[Foundation topics for electron microscopy](#)' lectures and must be taken by those wishing to use TEM/HRTEM/STEM instrumentation in their research. EM support staff will advise researchers on the lectures relevant to them. The course may also be taken for credit, see below.

Lecture 1: Electron diffraction: Ewald sphere, reciprocal space, indexing of crystals, Bragg law.

Lecture 2: Kinematical theory: Diffraction contrast, extinction distance, limitations of kinematical theory

Lecture 3: Dynamical theory of ED: Two beam equations, image contrast in the two-beam approximation, wave-mechanical approach, anomalous absorption.

Lecture 4: Phase contrast HRTEM: Overview, imaging theory, PCTF

Lecture 5: HRTEM II: Factors limiting resolution, Temporal and spatial coherence, simulation, Multislice approach.

Lecture 6: Scanning Transmission Electron Microscopy: Reciprocity, practical setup, imaging modes, coherent/incoherent imaging

Lecture 7: STEM II: Probe formation, Brightness, high-resolution imaging, the Ronchigram

Lecture 8: Aberration correction in (S)TEM: Lens aberrations, nomenclature, wave aberration-function, aberration-measurement, methods of correction, exit-waves. Implications for HRTEM and STEM.

Pre-requisites: [Foundation topics for electron microscopy](#) lecture course.

Postgraduate Assessment

Students seeking credit for the course should attend a minimum of 6 of the 8 lectures, and answer a set of problems and questions based on the topics covered in the lectures.

Further Reading

Williams, D. B. & Carter, C. B., **Transmission Electron Microscopy**, Plenum, chapters 6 (electron lens), 11-19 (diffraction), 22-25 (imaging), 27-28 (HREM), 29 (image simulation)

Reimer, L., **Transmission Electron Microscopy**, Springer-Verlag, chapters 2, 3 (electron optics), 6 (image contrast), 7 (kinematic and dynamical theory of ED), 8 (diffraction contrast)

Hirsch, P. B., Howie, A., Nicholson, R. B., Pashley, D. W., & Whelan, M. J., **Electron Microscopy of Thin Crystals**, R E Krieger Publishing

Spence, J. C. H., **High-Resolution Electron Microscopy**, Oxford Science Publications chapters 2, 3 (electron optics), 5 (HREM theory), 10 (HREM parameter measurement)

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 10 online lectures provide introductions to key topics within atomistic modelling, including crystallography, geometry optimization, running in parallel, electronic properties, EELS, vibrational properties and magnetism. The lectures are accompanied by self-paced exercises. Support is provided through weekly live sessions (weeks 3-7) with the course organisers. The student will then be asked to carry out their own computational study of a material and write up their results as a report, which will be used as the basis for the assessment of this course.

Course structure and requirements:

The practical work will be carried out on departmental-based servers running Linux with the CASTEP DFT software pre-installed. The student will be required to log onto the servers remotely, from their own computer. The course assumes familiarity with undergraduate level electronic structure and solid-state physics, and some experience in programming e.g. Matlab, Python. In the case that the course is oversubscribed, priority will be given to students who can demonstrate plans to use the methodology in their own research.

Modular Courses in Electron Microscopy

1. WDS and Quantitative X-ray Analysis

Module Co-ordinator: Dr C.J. Salter

Pre-requisites: Course open to provisional or approved users of SEMs who require to use EPMA techniques in the Department. Participants will be expected to be current users of EDX hardware. Attendance of the following postgraduate lecture courses (or relevant parts of, to be advised by EM support staff): [‘Foundation topics in electron microscopy’](#) and [‘Spectroscopy with the \(S\)TEM’](#).

Given by: C.J. Salter

Description: Two one-hour lectures plus about 9 hours of practical instruction and practice

Aim: To give potential microprobe users basic knowledge of practical qualitative and quantitative WDS analysis so that that can understand how data produced by the machine was obtained and the limitation of such data. As such anyone wanting to have work carried out on the JXA8800 should attend this course. The course also covers the methodology required to carry out quantitative X-ray analysis using Energy Dispersive Spectrometers.

Course Structure:

Lectures: Understanding of X-ray generation . K, L, M lines shape and intensity (in comparison to EDX), relationship between accelerating voltage, critical X-ray excitation energy, X-ray intensity and X-ray generation volume.

X-ray detection using WDS: Rowland’s Circle, Bragg’s Law, pulse height detector, dead-time, counter types, n-th order lines, the limited range of specific crystals, detector geometry.

Matrix effects: Atomic number, absorption and fluorescence effects, geometry.

Data acquisition: Qualitative - spectral, line and area techniques, nature and sources of errors, counting and sampling statistics, detection limits; semi-quantitative - appropriate use and limits of quantification; Quantitative - the nature use of primary and secondary standards, peak and background overlap corrections and deconvolution. Correction methods ZAF, PhiRhoZ, calibration curve, thin film, and Monte Carlo Methods.

Presentation of results.

Simple image processing and analysis. Common practical problems: sample preparation, sample charging, carbon coating. Analysis of thin films on solid substrates.

Practicals: Demonstration of Loading specimens. Selection of appropriate conditions for analysis. Acquisition of a full WD spectrum: elemental identification, identification of nature and scale of interference and overlap problems. The acquisition line and area data. Processing of linear and area data, including plotting phase analysis from images, and limited image processing and analysis. Demonstration of acquisition of standard data. The setting up of analysis points using beam and stage movement methods.

Outcome: It is necessary for anybody intended to use JXA8800 to attend this course so that they understand how any microprobe results were obtained, the statistical, chemical and spatial limitations of those results. However, the course is not intended to train the participant to approved user status; that will require further one to one training.

Assessment: Simple tests using various samples will be set for each technique.

Frequency: Trinity Term (possibly repeated if sufficient demand)

Further Modules: Required for approved user status (by arrangement):

- Qualitative analysis – line and area
- Quantitative analysis – acquisition
- Data processing
- Acquiring standards

Further Reading

Scott, V.D. & Love, G., **Quantitative Electron-Probe Microanalysis**, Ellis Horwood

Giannuzzi, L.A., & Stevie, F. A., **Introduction to Focused Ion Beams: instrumentation, theory, techniques and practice**, Springer

2. Electron Back Scattered Diffraction (EBSD)

Module Coordinator: Dr P. Karamched

Pre-requisites: Course open to provisional or approved users of the Zeiss EVO or who require to use EBSD facilities in the department.

Given by: G.M. Hughes, P. Karamched

Description: Two one-hour lectures covering the basic principles of EBSD and analysis of EBSD data, plus approximately six hours of practical instruction and practice.

Aim: To give inexperienced users a basic knowledge of practical EBSD.

Course Structure: (Features in brackets are described but not taught as part of this course.)

Lectures: Formation of EBSD patterns: backscattering of electrons by solids, structure factors, (intensity profiles across Kikuchi band requires dynamical diffraction theory). Indexing EBSD Patterns: Pattern centre, Gnomonic projection, angles between diffracting planes, orientation measurement, the Hough transform, automated analysis. Data Analysis: pole figures, inverse pole figures, (Euler angles and Orientation Distribution Functions), misorientations, disorientations, matrices, axis/angle pairs (RF vectors, quaternions), coincident site lattice. Orientation mapping, enhancing/filtering maps. Spatial and angular resolution.

Practicals: TSLOIM EBSD mapping software. Specimen loading and geometry. Input of sample details - crystal phases present, macroscopic reference axes. Appropriate microscope settings - beam energy, beam current, magnification. Appropriate EBSD camera settings - binning, exposure time, video gain, 'flat fielding'. Appropriate Index Algorithm settings - number of bands to index, angular tolerance. Verifying automated analysis results. Setting up and running an orientation map. Data Analysis.

Outcome: Course participants will learn the basics of EBSD, and its limitations. They will be trained: how to obtain EBSD patterns, how to perform automated crystal orientation mapping and when to seek help with more difficult analysis problems.

Assessment: Individual practical assessment.

Frequency: Michaelmas Term (possibly repeated if sufficient demand).

3. Focussed Ion Beam milling

Module co-ordinator: Dr G.M. Hughes

Given by: G.M. Hughes

Description: Two one-hour lectures and two to three three-hour practical training sessions.

Lecture 1:

Background to FIB. Liquid metal ion sources. Optical design. Ion-sample interaction and sputtering. Imaging and contrast mechanisms – secondary electron and ion imaging. Ion milling and implantation. Ion beam resolution and profile.

Lecture 2:

Applications of FIB. Gas injection system for enhanced milling and deposition. Sample preparation. Ion beam damage. General applications overview, followed by general discussion/workshop about the attendees' projects – how to approach their problem.

Practical Sessions:

1. Introduction to the instrument. Mounting and loading samples. Turning on and off the Ga ion source. Basic imaging, setting sample to the eucentric height. Focusing and correction of astigmatism. Basic milling operations.
2. Application based session, dependent on attendees – e.g. cantilever fabrication, TEM sample prep.
3. Individual sessions where the user will practice sample exchange, setting up and working on the instrument toward their application.

Outcome: Trainees should become competent users of the FIB system and capable of carrying out basic milling / deposition specific to their application.

Assessment: During the first session trainees are demonstrated loading and unloading specimens, turning on and off the system and using the gas injector needles. Upon reaching a standard whereby the machine can be used safely, the user will be granted approved status.

Frequency: Termly

Pre-requisites: Those attending the module will be required to take part in basic SEM training prior to the start date if they do not already have SEM experience.

4. Advanced Microanalysis

Module Co-ordinator: Dr N.P. Young

Given by: S. Lozano-Perez

Pre-requisites: Experienced (S)TEM users with existing knowledge of EELS and EDX (e.g. EDX module, EELS module, STEM module). Approved users of Jeol 3000F or Jeol 2200FS or ARM 200F. Attendance of the following postgraduate lecture courses (or relevant parts of, to be advised by EM Facility): [‘Spectroscopy with the \(S\)TEM’](#).

Description: A one-hour lecture plus about six hours of practical instruction and practice.

Aim: To ensure that (S)TEM users in this department use the different microanalysis techniques efficiently and are up to date with the latest trends.

Course Structure:

Review of all microanalysis techniques available in the department

Quick review of EDX, EELS and HAADF: advantages and disadvantages

Approaches to elemental mapping:

EDX Spectrum Imaging

EELS Spectrum Imaging

EELS Image Spectroscopy

How to improve spatial resolution

How to improve SNR

Microscope’s suitability with advantages and disadvantages

Optimizing acquisition and processing: Using Digital micrograph scripting language

Benefits of simultaneous acquisition of different signals

Practicals: Hands-on sessions in the Jeol ARM or on the dedicated computers in the EM lab to demonstrate the concepts covering in the lectures, including:

- Optimization of EFTEM acquisition
- STEM alignment for EDX and EDX/EELS/HAADF simultaneous acquisition
- Demonstration of related Digital Micrograph scripts

Outcome: Course participants will be aware of the potentiality of the facilities in the department and they will use them efficiently. This course will enable some researchers to become advanced users who will further develop these techniques.

Assessment: Some standard samples will be used to demonstrate the potential of the various techniques and their associated artefacts. Course attendants will be asked about the quality/suitability of different results and to explain the origin of the artefacts.

Frequency: Annually, Trinity Term

5. Analysis of HREM Images

Module Co-ordinator: Dr N.P. Young

Given by: N.P. Young

Pre-requisites: Course open to HREM users. Participants will already have significant experience in HRTEM and/or obtained focal-series data with Dr Young or others.

Attendance of the following postgraduate lecture courses (or relevant parts of): ['Imaging & Diffraction in \(S\)TEM'](#).

Description: Two one-hour lectures plus about 4 hours of practicals.

Aim: To allow FEGTEM and HREM users in this department to interpret properly their HREM images and to calculate the exit-wavefunction.

Course Structure:

Lectures: on Image Simulation and Exit-wave restoration

Practicals: Hands-on sessions using JEMS multislice image simulation and FTSR exit-wave restoration software

Outcome: Course participants will be aware of the need to interpret HREM images correctly, and know how to use the basic software to do this.

Assessment: Individual.

Frequency: Hilary (possibly repeated if sufficient demand)

Third Year Undergraduate Options

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.

Materials & Devices for Optics & Optoelectronics

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

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.

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
 - Nb₃Sn 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.

Microstructural Control in Engineering Alloys

Aluminium Alloys (4 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: high strength and toughness.
- HSLA Steels: thermomechanical treatments to control carbides.
- Stainless steels: FeCrNi family 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.
- Beta alloys: designed for trade-off between strength and fracture toughness.
- Intermetallics: TiAl system as used in GENX engine; processing route; order-disorder reactions.
- Oxidation resistance of titanium.

Magnesium Alloys (2 lectures)

- Cast Alloys, Wrought Alloys, Future opportunities

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

G. Krauss. **Steels processing, structure and performance**.

Bhadeshia, H. K. D. H. **Bainite in Steels: Theory and Practice** (3rd edition).

D.T. Llewellyn and R.C. Hudd. **Steels Metallurgy and Applications**, 1992, Butterworth-Heinemann.

F.H. Froes. **Titanium Physical Metallurgy Processing and Applications**. ASM International, 2015.

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.
- a. Biomechanics.
 - a) the joint reaction force.
 - b) device design.
- b. Drug delivery devices – liposomes, natural polymers and artificial polymer based systems.
- c. Tissue expanders. Use in plastic and reconstructive surgery.
- d. 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.

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 lascc.**" 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 (Rpv) 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.

tbc

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.

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
 - a. Polymer blends
 - b. Polymer films
 - c. Reflectivity techniques
 - d. 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

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-](http://library.lanl.gov/cgi-bin/getfile?00326651.pdf)

[bin/getfile?00326651.pdf](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.

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)

- Introduction to quantum computing and quantum error correction
- Superconducting circuits
- Trapped ions and cold atoms
- Topological qubits
- Semiconductor quantum dots
- Colour centres in wide gap materials
- Molecular systems

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>

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 electrolyzers/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).

Colloquia and Lecture Lists in Materials
and Other Physical Science Departments

Research Colloquia

Departmental Colloquia normally take place at 3.30pm on certain Thursday afternoons in weeks to be advised on our website – typically four in each of Michaelmas & Hilary Terms and two in Trinity Term. Coordinator – Lorraine Laird

A complete list of colloquia, including links to colloquia lists from other MPLS departments, will be available on the Departmental website

<http://www.materials.ox.ac.uk/news/colloquia.html>

In addition to the Departmental Colloquia, seminar series are organised by the Materials Modelling Laboratory (**MML Seminars**) and the Quantum Information Processing research groups (**QIP Seminars**).

Finally, each year a significant number of **ad hoc talks** are arranged by individual research groups and normally advertised by email.

Lectures in Other Science Departments

For up to date information on the lectures offered in Michaelmas Term by other Departments such as Mathematical Sciences, Engineering Sciences, Physics or Chemistry, please see the following website:

<http://www.ox.ac.uk/students/academic/lectures/>