



Materials Science (MS)
Final Honours School
Core Lecture Course Synopses
2022-23



Department of Materials



Materials Science (MS)

Final Honours School Core Lecture Course Synopses 2022-2023

Version	Action	Date
Version 1.0	Published in MT22	05/10/2022
-	-	-
-	-	-

General Paper 1: Lifecycle, Processing and Engineering of Materials	3
Selection and Production of Engineering Materials	6
Processing for Control of Materials Properties and Performance	9
Materials End-of-Life.....	13
General Paper 2: Electronic Properties of Materials	16
Electronic Structure of Materials	19
Semiconductor Materials and Devices.....	22
Magnetic Properties of Materials	24
Electrical and Optical Properties of Materials	26
General Paper 3: Mechanical Properties of Materials	28
Elastic Deformation of Materials	31
Plastic Deformation of Materials	35
Structural Failure of Materials	38
General Paper 4: Structure and Thermodynamics of Materials	43
Statistical Mechanics and Thermal Properties of Materials.....	45
Structural and Compositional Characterisation of Materials	48
Phase Transformations.....	51
Other Lectures.....	54
Maths - Partial Differential Equations & Fourier Series and Tensors	55

General Paper 1: Lifecycle, Processing and Engineering of Materials

General Paper 1: Lifecycle, Processing and Engineering of Materials

Summary

This paper considers the whole life-cycle of materials. It begins by introducing materials selection processes such as selection diagrams, and figures of merit/optimization parameters, and considers the wide range of parameters that might be of importance (mechanical, electrical, optical etc. properties, cost, disposal, lifetime and toxicity, materials abundance). Examples are used to give a broad overview of material types, how they relate and compete with one another, and how engineering decisions on materials selection are made.

The manufacture of materials (alloys/ceramics/polymers and their composites) is then considered, and key topics of materials preparation from extraction metallurgy, powder preparation and polymer synthesis are addressed. Emphasis is placed on the control of the materials characteristics, including additives & contaminants, and properties of the resulting materials, using example cases that are discussed within their engineering context.

The links between materials processing and engineering properties are considered, with a focus first on thermal and chemical treatments, using examples include the role of quenching and annealing/sintering, and then mechanical treatments where flow and plastic deformation during processing are used to optimise materials properties and to control and exploit the anisotropy that may be introduced by this in monolithic and composite materials. The criteria for yield in metals and polymers are introduced and applied in the context of macroscopic deformation in materials processing.

Finally, some important mechanisms that limit the lifetime of materials are considered, mainly in the context of environmental degradation of metals and polymers, and how this may be protected against. This leads to a consideration of materials sustainability and the recycling of materials at end of life.

Lifecycle and Processing of Materials comprises three sections

- Selection and Production of Engineering Materials (10 lectures)
- Processing for Control of Materials Properties (16 lectures)
- Materials end-of-life: Environmental degradation and recycling (12 lectures)

Selection and Production of Engineering Materials

Overview

Building on the introduction in the Prelims course to the general materials types, properties and relationship to structure, bonding and chemistry, this course provides a more detailed examination of the choices a typical materials engineer would make in selecting specific materials and their combination as well as a description of how the various materials are synthesised, extracted and produced. The opportunity is taken to address materials selection 'in the round' covering all materials types together and seeking to provide, where possible, a quantitative and holistic approach to materials selection, considering a wide range of parameters for structural and functional materials, as well as the economics and pointing the way to lifecycle aspects of materials selection which will be covered in detail in the third block of lectures within this paper.

Materials Selection (4 lectures) Michaelmas Term

Overall materials classes

- Summary of key properties of materials classes
- Examples of different materials types and properties including alloys of iron, light alloys, polymers, ceramics.

Engineering decision-making for materials selection

- Materials selection diagrams.
- Figures of merit for combining the effects of several materials parameters.
- Composite materials (explore matrix types, typical properties and reinforcement types)
- Composites: another option in materials selection
- Matrix classes – value added in making composites vs. use of matrix material alone
- Additive types – 2D, 1D and particulates.
- Hierarchical structures

- Interfacial bonding
- Additives and formulations

Production of Base Materials (6 lectures) Trinity Term

Alloys

- Steelmaking: basic oxygen furnace, electric arc furnace, secondary steelmaking, control of C, Si, Mn, P & S in steel.
- Stainless steels: compositions effects and alloying additions.
- Aluminium: production and properties, overview and classifications of the alloy types.
- Titanium: extraction and alloys.

Ceramics

- Powder production
- Particle shape and size distribution
- Comparison with metal and polymer powders

Polymers

- Synthesis by step-growth and chain growth, including radical and ionic synthetic routes.
- Polymerization processes – bulk, solution, suspension and emulsion
- Stereochemistry and control during synthesis, copolymers
- Characterisation of synthesized materials: molecular weight, stereochemistry and composition
- Biopolymer ‘synthesis’: Cellulose, PHB, hierarchical structures in natural materials

Composites

- Composites manufacture – Combining materials: PMCs, MMCs, & CMCs, Cermets, particulate and nanocomposites.
- Control of distribution and orientation of reinforcement and matrix infiltration.

Further reading

Ashby, M. F. and David R. H. Jones. **Engineering Materials 1 [Electronic Resource] : An Introduction to Properties, Applications, and Design.** 4th edition, Butterworth-Heinemann, 2012. Engineering Materials One.

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.

Ashby, M. F. **Materials Selection in Mechanical Design**. Fifth edition, Butterworth-Heinemann, 2016.

Ashby, M. F. and Kara Johnson. **Materials and Design: The Art and Science of Material Selection in Product Design**. Third edition, Butterworth-Heinemann is an imprint of Elsevier, 2014. Ebook Central. Online.

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

Cowie, J. M. G. and V. Arrighi. **Polymers : Chemistry and Physics of Modern Materials**. 3rd edition, CRC, 2007. Dept. of Materials Library 45 COW/1. Chapters 1-4, 9.

Ghosh, Ahindra. **Secondary Steelmaking: Principles and Applications**. CRC Press, 2001. Dept. of Materials Library Overnight 51 GHO.

Hull, Derek and T. W. Clyne. **An Introduction to Composite Materials**. Second edition, Cambridge University Press, 1996. Cambridge Solid State Science Series. Online. chapters 2,3, 7, 12.

Kumar, Anil and Rakesh K. Gupta. **Fundamentals of Polymers**. McGraw-Hill, 1998. Mcgraw-Hill Chemical Engineering Series. Dept. of Materials Library 45 KUM. chapters 1-8.

Russell, Alan M. and Kok Loong Lee. **Structure-Property Relations in Nonferrous Metals**. Wiley-Interscience, 2005. Dept. of Materials Library Overnight 52 RUS.

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

Lütjering, G. and J. C. Williams. **Titanium**. 2nd edition, Springer, 2007. **Engineering Materials and Processes**. Online.

Matthews, F. L. and R. D. Rawlings. **Composite Materials: Engineering and Science**. Chapman & Hall, 1994. chapters 2-5, 10.

Polmear, I. J. **Light Alloys : Metallurgy of the Light Metals**. 3rd edition, Arnold, 1995. Metallurgy and Materials Science. Dept. of Materials Library 52 POL/F or 52 POL/H.

Walton, David J. and J. Phillip Lorimer. **Polymers**. Oxford University Press, 2000. Oxford Chemistry Primers ; 85. Dept. of Materials Library 45 WAL. chapters 1-4.

Processing for Control of Materials Properties and Performance

Overview

This course focusses on the role of heat, chemistry and mechanical deformation during materials processing and manufacture of components, in determining structure, properties and performance of materials. The course is structured to take the opportunity to compare and contrast across different materials classes while introducing key concepts in turn, such as high temperatures to allow diffusive processes, chemical processes during processing, or control an exploitation of anisotropy that can be induced during processing.

Introduction.

- Classification scheme for materials processes, and processing in the context of materials types.
- Relationship between processing and design.
- Cost modelling
- Modern trends: numerical analysis by process modelling; additive manufacturing to complement subtractive manufacturing.

Shaping processes involving casting and moulding

- Metals vs polymers.
- Importance of heat management. Heat transfer: interfacial resistance vs conduction.
- Roles of fluidity (metals) and rheology (polymers) emphasising shear thinning and extensional flow.
- Examples: processing of glass and its toughening; continuous casting of steel; injection moulding of polymers and related processes; pressure die casting; Bridgeman processing – nickel superalloys vs Czochralski growth of silicon; anisotropy and its advantages/disadvantages.

Heat Treatment

- Traditional ceramics.
- Aluminium alloys vs magnesium alloys.
- Steel: normalising vs quench/tempering; the concept of hardenability.
- The role of surface conditioning: anodisation and phosphate coatings for Al alloys, carburising/nitriding for steels.
- Welding and joining processes; the importance of microstructural evolution. Defect control, residual stresses and distortion; the importance of heat treatment for remedial purposes.

Deformation processing

- Macroplasticity: true stress, true strain and yielding.
- Stress-strain relationships for elastic-plastic materials.
- Tresca, Von Mises and Coulomb yield criteria. Application of yield criteria: yielding in torsion and compression.
- Plastic instability: Considere's criterion.
- Applications of macroplasticity: forging, rolling, drawing and extrusion.
- Case studies: drawing of metal wires, open die forging, extrusion of polymers, controlled rolling of steel.

Powder processing

- Powder processing methods.
- Powder production methods, e.g. atomisation, mechanical attrition.
- Closed die compaction, sintering, hot pressing, hot isostatic pressing (HIP) and cold isostatic pressing (CIP) as applied to metals, hard metals, intermetallics, ceramic and pharmaceutical powders.
- Sintering: mechanisms of deformation, densification and grain growth. Sintering maps.

Processing of hybrid structures

- Technological incentives. Laminates, trusses, foams, reinforcement.
- Production methods for metal matrix, ceramic matrix and polymer matrix composites.
- The principles of stress analysis, heat transfer, chemical reaction at surfaces.
- Challenges: anisotropy, joining.

- Examples: honeycombs in Al. Superplastic forming of hollow Ti structures. GLARE for aircraft fuselages. AM-manufactured synthetic bone. Concrete: reinforced and pre-stressed, with emphasis on cement processing.

Additive manufacturing

- Example case studies

Further reading

Ashby, M. F. **Materials and the Environment : Eco-Informed Material Choice.**

2nd edition, Elsevier/Butterworth-Heinemann, 2013. Dept. of Materials Library Overnight 57 ASH/1.

Ashby, M. F. et al. **Materials : Engineering, Science, Processing and Design.**

Fourth edition, Butterworth-Heinemann, an imprint of Elsevier, 2019.

Asthana, R. et al. **Materials Processing and Manufacturing Science.** Boston: Elsevier Academic Press, 2006. Ebook Central.

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

Dieter, George E. **Mechanical Metallurgy.** 3rd edition, McGraw-Hill, 1986. McGraw-Hill Series in Materials Science and Engineering.

Doremus, Robert H. **Glass Science.** 2nd edition, Wiley, 1994. Dept. of Materials Library Overnight 44 DOR.

Fredriksson, Hasse and Ulla Akerlind. **Solidification and Crystallization**

Processing in Metals and Alloys. Wiley, 2012. Dept. of Materials Library 30 FRE.

Hosford, William F. and Robert M. Caddell. **Metal Forming: Mechanics and**

Metallurgy. 4th edition, Cambridge University Press, 2011. Dept of Materials Library 50 HOS/2.

McCrum, N. G. et al. **Principles of Polymer Engineering.** Oxford University Press, 1988. Oxford Science Publications. Dept. of Materials Library 45 McC/3A.

Porter, David A. et al. **Phase Transformations in Metals and Alloys.** 3rd ed.

edition, CRC; Taylor & Francis [distributor], 2009. Dept. of Materials Library 53 POR/I.

Poirier, D. R. and G. H. Geiger. **Transport Phenomena in Materials Processing.**

Minerals, Metals & Materials Society, 1994. Dept. of Materials Library Overnight 50 POI/A.

Polmear, I. J. **Light Alloys: From Traditional Alloys to Nanocrystals**. Fourth edition, Elsevier Butterworth-Heinemann, 2006. Dept. of Materials Library 52 POL/J.

Richerson, David W. **Modern Ceramic Engineering: Properties, Processing, and Use in Design**. Fourth edition, CRC Press, 2018.

Reed-Hill, Robert E. and R. Abbaschian. **Physical Metallurgy Principles**. 3rd. edition, PWS-Kent Publishing Co., 1992. The Pws-Kent Series in Engineering. Dept. of Materials Library 50 REE/D.

Reed, Roger C. **The Superalloys: Fundamentals and Applications**. Cambridge University Press, 2006. Dept. of Materials Library 52 REE.

Taylor, H. F. W. **Cement Chemistry**. 2nd edition, Thomas Telford, 1997.

Thümmeler, F. and R. Oberacker. **An Introduction to Powder Metallurgy**. Institute of Materials, 1993. Institute of Materials Series on Powder Metallurgy; Bk. 490. Dept. of Materials Library 55 THU.

Materials End-of-Life

Overview

This course introduces the concept of lifecycle of materials, focussing on their end-of-life: degradation and recycling. Degradation is ultimately responsible for materials reaching their end-of-life, changing their mechanical and physical properties and, ultimately, their performance. The most common form is environmental degradation where materials deteriorate as a result of interacting with their environment, particularly if oxygen or hydrogen are involved (corrosion). Corrosion and protection of metals will be covered in detail in this section. Polymers degradation will also be covered, focusing on the effect of light and bio-organisms. Both groups of materials can contribute to a more ecologically sustainable world if recycled and re-used properly. This will be the focus of the last part of this group of lectures on sustainability and recycling.

The concept of lifecycle is first introduced as a way of maximising the efficiency of product manufacturing and minimising the impact to the environment. A product cycle starts during mining/extraction of raw materials from the earth and ends when the same materials are either reused, recycled, recovered or discarded. With the aim on reducing waste, the concept of sustainability is introduced and the product life cycle explained.

Introduction to Lifecycle of Materials (1 lecture)

Sustainability and recycling (3 lectures)

Metals sustainability

- Recycling steel, Al and Cu

Polymers sustainability

- Recycling plastics
- Case studies on lifecycle of materials

Environmental Degradation and Protection (8 lectures)

Introduction to environmental degradation of materials

Corrosion and protection

- Introduction
- Basic concepts (revision): Polarisation; Tafel lines; Evans diagrams; Pourbaix diagrams
- Passivity
- Forms of corrosion: Uniform; Localised: Galvanic, crevice and pitting corrosion
- Importance of environment
- Corrosion prevention: Materials selection; Altering the environment; Inhibitors; Design; Cathodic and anodic protection; Coatings and paints

Polymer degradation and protection

Further reading

Ashby, M. F. **Materials and the Environment : Eco-Informed Material Choice.**

2nd edition, Elsevier/Butterworth-Heinemann, 2013. Dept. of Materials Library Overnight 57 ASH/1. chapters 1-10.

Ashby, M. F. et al. **Materials and Sustainable Development.** Butterworth-Heinemann, 2015. (2016 online). Dept. of Materials Library 57 ASH/2. chapters 1-3, 8, 13, 14.

Fontana, Mars G. **Corrosion Engineering.** 3rd edition, McGraw-Hill, 1986. McGraw-Hill Series in Materials Science and Engineering. Dept. of Materials Library 43 FON/A.

Goodship, Vannessa. **Introduction to Plastics Recycling.** 2nd edition, Smithers Rapra, 2007. Dept. of Materials Library Overnight 57 GOO.

Gorgolewski, Mark. **Resource Salvation: The Architecture of Reuse.** Wiley-Blackwell, 2018. Ebook Central. Online. chapters 1, 2, 4.

Jones, Denny A. **Principles and Prevention of Corrosion.** 2nd edition, Prentice Hall, 1996. Corrosion. Dept. of Materials Library 43 JON.

Rogoff, Marc. **Solid Waste Recycling and Processing,** 2nd Edition. 2nd edition, William Andrew, 2013. Online. chapters 1,4 ,5.

Scott, Gerald. **Degradable Polymers : Principles and Applications**. 2nd edition, Kluwer Academic Publishers, 2002. Dept. of Materials Library 45 SCO.

Scully, J. C. **The Fundamentals of Corrosion**. 3rd edition, Pergamon, 1990.

International Series on Materials Science and Technology (Merlin Books). Dept. of Materials Library Overnight 43 SCU/1E.

Trethewey, Kenneth R. and John Chamberlain. **Corrosion for Science and Engineering**. 2nd edition, Longman Scientific & Technical, 1995.

West, J. M. **Basic Corrosion and Oxidation**. Horwood, 1980. Dept. of Materials Library 43 WES/2A or 43 WES/2B.

General Paper 2: Electronic Properties of Materials

General Paper 2: Electronic Properties of Materials

Summary

This paper considers the electronic properties of a wide range of different classes of materials. Many materials, and electronic materials in particular, can have anisotropic properties that relate causes (e.g. electric field) and effects (e.g. electric current) in different directions. So, the course depends on the introduction to Tensors in the Mathematics course, which provides the foundations for describing this anisotropic behaviour in crystal systems.

The course builds up the theory of electronic structure using principles introduced in the first year quantum mechanics course, since the electronic structure of materials is fundamental not only to the electrical properties of materials but also their optical and magnetic properties and also many aspects of their mechanical and thermal properties.

The important class of semiconductors is then considered, including both inorganic and organic (polymer) semiconductors which are critical for the production and control of electrical and optical signals in computation, optical communications and the production of light, and also solar cells for energy generation. The course shows how quantum and statistical mechanics are used to understand the response of materials to magnetic fields, and why certain materials form permanent magnets. The theory of magnetic domains, and the experimental techniques used to analyse magnetic materials, are introduced and technologically important magnetic materials are reviewed. Superconducting materials and their properties are covered.

Electrical and optical properties of materials, and their practical applications, are addressed, including the conductivity of materials that are normally considered insulators, the polarisability of materials in electric fields and superconductivity. The relationship between electrical and optical properties is developed using Maxwell's equations.

Electronic Properties of Materials comprises three sections

- Electronic Structure of Materials (12 lectures)
- Semiconductor Materials and Devices (10 lectures)
- Magnetic Properties of Materials (10 lectures)
- Electrical & Optical Properties of Materials (8 lectures)

Electronic Structure of Materials

Overview

Electronic structure of materials concerns the question “what are the allowed states of electrons in a material, and which ones are occupied under what conditions?” It is fundamental not only to the electrical properties of materials but also their optical properties and many aspects of their mechanical, thermal, optical and magnetic properties. This course builds up the theory of electronic structure using and expanding principles introduced in the first year quantum mechanics course. The first part of the course concerns the electronic structure of atoms and molecules. The remaining part focuses on crystalline materials, starting with the free electron model before introducing translational symmetry, Brillouin zones and band structure, distinguishing the cases of metals, semiconductors and insulators. Different models of electronic structure are introduced and illustrated with examples. Discussing electron motion in semiconductors leads to the introduction of the concepts of holes and effective mass. The course concludes with an assessment of the strengths, weaknesses and range of applicability of the different models.

- Recap of key quantum mechanics concepts from the Prelims course
- Angular momentum: operators, quantum numbers and commutation relations
- Electrons in atoms: single-electron atoms and central field model for many-electron atoms. Aufbau and Pauli principles and the structure of the periodic table
- Electrons in molecules: H₂ molecule in the tight-binding approximation, bonding and antibonding states. Concepts of molecular orbitals, HOMO and LUMO and density of states
- Response of electrons to external stimuli: perturbation theory, Fermi's golden rule and selection rules. Introduction to Dirac notation. Examples

of experiments probing electronic structure, e.g. photoemission and optical absorption

- Free electron theory - Density of states in one, two and three dimensions,
- Fermi energies, Fermi wavevectors and Fermi surfaces. DoS at the Fermi energy. Calculating Fermi energies from electron densities.
- Fermi-Dirac distribution, electronic specific heat and electrical and thermal conductivity.
- Band theory -general principles: periodic lattices and Bloch's theorem, Brillouin zones and reciprocal lattice. Number of electrons per band. 2D square lattice for monovalent, divalent and trivalent materials.
- Band Theory -NFE approximation: NFE secular equation, band structure and density of states of simple metals.
- Band theory -TB approximation: TB secular equation, simple example lattices.
- Band structure of sp-valent semiconductors and d-valent transition metals, direct and indirect band gaps
- Motion of electrons in semiconductors: concepts of holes. Effective mass

Further reading

Eisberg, Robert Martin and Robert Resnick. **Quantum Physics of Atoms, Molecules, Solids, Nuclei, and Particles**. 2nd edition, Wiley, 1985. Chapters 7, 8, 9, 12, 13.

Hook, J. R. and H. E. Hall. **Solid State Physics**. 2nd edition, Wiley, 1991.

Manchester Physics Series. online. Chapters 3, 4, 5.

Ibach, H. and H. Lüth. **Solid-State Physics : An Introduction to Principles of Materials Science**. Springer Berlin Heidelberg : Imprint: Springer, 2009. Online. Chapters 1, 6, 7, 9, 12.

Kittel, Charles and Paul McEuen. **Introduction to Solid State Physics**. Global edition, Wiley, 2018. Kittel's Introduction to Solid State Physics. Chapters 6, 7, 8

Pettifor, D. G. **Bonding and Structure of Molecules and Solids**. Clarendon Press, 2002. Oxford Science Publications. Chapters 3, 5, 6, 7.

Rae, Alastair I. M. and Jim Napolitano. **Quantum Mechanics**. Sixth edition, CRC Press, Taylor & Francis Group, 2016. Ebook Central. Online. Chapters 8-10.

Singleton, John. **Band Theory and Electronic Properties of Solids**. Oxford University Press, 2001. Oxford Master Series in Condensed Matter Physics. Dept. of Materials Library 21 SIN. Chapters 1-6.

Semiconductor Materials and Devices

Overview

Semiconductors are a key component in enabling the technological world in which we live. They provide the ability to control electrical signals so allowing, for example, computation and their optical properties allow the emission of light which is used in lighting (LEDs), lasers and optical communications. The absorption of light is used in solar cells which are predicted to become the major carbon free energy source on the planet. This lecture course gives an overview of why some materials are semiconductors and the characteristics of the charge carriers they contain. The course moves on to describe the junction between n- and p-type material which has asymmetric current characteristics and forms the basis of most electronic devices. In the second half of the course the emphasis is on the engineering applications of semiconductor materials with descriptions as to how they may be used to produce devices such as transistors, memory devices, lasers and solar cells.

- Brief review of band diagrams. Donor and acceptor levels, defect states.
- Electron and hole statistics, carrier concentration, temperature dependence, intrinsic and extrinsic materials. Majority and minority carriers.
- Current flow, drift, mobility, conductivity, Hall effect.
- Minority carrier effects, diffusion, recombination, lifetime, diffusion length.
- P-N junctions, band bending, depletion region, I-V characteristics.
- Metal-semiconductor contacts, Schottky barrier, ohmic contacts.
- Diode devices; switches and microwave oscillators
- Transistors: bipolar, MOSFET, MESFET, HEMT, OFET.
- Optical devices: Photodetectors, solar cells, light emitting diodes, lasers.
- Semiconductor memory devices: SRAM, DRAM, CCDs

Essential reading

Solymar, L. et al. **Electrical Properties of Materials**. Tenth edition, Oxford University Press, 2018. Oxford Scholarship Online. Online. Chapters 8 and 9.

Further reading

Böer, Karl W. **Semiconductor Physics**. Springer International Publishing : Imprint: Springer, 2020

Fiore, James. **Semiconductor Devices: Theory and Application**. dissidents, 2018. Library Open Textbook. Online.

Neamen, Donald A. **Semiconductor Physics and Devices**. 4th edition, McGraw-Hill Higher Education ; McGraw-Hill [distributor], 2011.

Sze, S. M. and Kwok Kwok Ng. **Physics of Semiconductor Devices**. 3rd edition, Wiley-Interscience, 2007. Ebook Central. Online.

Magnetic Properties of Materials

Overview

The course shows how the combination of quantum and statistical mechanics is needed to understand the response of materials to magnetic fields, and why certain materials form permanent magnets. The theory of magnetic domains will be discussed to understand why for example iron and steel can be made into permanent magnetic, but not all objects made from iron or steel are magnetic. The second half of the course addresses the phenomena of superconductivity; the ability of certain materials to support an electric current without dissipation.

Superconductors can be used to create magnetic fields (e.g. in MRI machines) – however, we shall see that these two topics are also linked at a more fundamental level.

Background

- Recap of magnetic materials: useful definitions and equations. Concept of magnetic energy.
- Quantum mechanics of isolated atoms. Spin, orbital angular momentum, S-O coupling, Hund's Rules

Microscopic theory of Magnetic Materials

- Langevin Theory of Diamagnetism
- Curie Paramagnetism: Statistical mechanics of a spin-half paramagnet. Orbital and Spin magnetic moments. Lande g-factor.
- Ferromagnetism: Curie-Weiss Theory
- Anti-ferromagnetism and Ferrimagnetism
- Magnetic Properties of Metals: Pauli Paramagnetism. Ferromagnetism of 3d metals.
- Magnetic Domains

Superconductivity

- Meissner Effect: expulsion of magnetic field, difference to perfect conductor.
- Overview of BCS Theory (Role of phonons, Cooper pairs, Superconducting gap)
- Thermodynamics of the superconducting state
- Surface Energy –Type I vs. Type II superconductors
- High-Temperature Superconductivity

Further reading

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

Kittel, Charles and Paul McEuen. **Introduction to Solid State Physics**. Global edition, Wiley, 2018. Kittel's Introduction to Solid State Physics. Many editions: all good.

Narlikar, A. V. **Superconductors**. Oxford: Oxford University Press, 2014.

Solymar, L. and D. Walsh. **Electrical Properties of Materials**. 6th edition, Oxford University Press, 1998. Materials Dept. Library 21 SOL/Q. Many editions: all good.

Spaldin, Nicola A. **Magnetic Materials: Fundamentals and Applications**. 2nd edition, Cambridge University Press, 2010. Ebook Central. Online. 1st or 2nd edition both good.

Electrical and Optical Properties of Materials

Overview

This lecture course reviews the electrical and optical properties of materials, building on the first year Electromagnetic Properties and Devices course and introducing more complex ideas such as anisotropic behaviour and frequency-dependence. It begins by looking at the mechanisms for electrical conductivity in materials normally considered insulators, including ionic crystals, polymers and high temperature superconductors. Polarizability of dielectric materials in an electric field is then explored, with a focus on different polarisation mechanisms and frequency dependence. Ferroelectric materials are revisited, with an emphasis on key electroceramic compounds used in device applications. The relation between electrical and optical properties is developed using Maxwell's equations. Examples of the application of materials' electrical and optical properties to practical devices are given throughout the course.

Electrical conductivity of materials with different types of bonding.

- Metals, semiconductors and insulators
- Ionic crystals: intrinsic & extrinsic vacancy density; energies of formation & activation; self-diffusion; ionic conductivity; superionic conductors; application of ionic conductors in solid state battery electrolytes; electron hopping conductivity.
- Polymers: as insulators, semi-conductive polymers, composite conductivity and ionic conductivity.
- High Temperature Superconductors: effect of electron/hole doping on transition temperature; electronic phase diagrams.

Dielectric Properties

- Lorentz field, Clausius-Mossotti relation.
- Types of polarisation: electronic, ionic, orientation, space- charge.
- Static permittivities of gases, liquids and solids.

- Frequency dependent polarisation in non-polar and polar substances: real and imaginary components of dielectric constant; resonant and weak absorption cases; dielectric losses
- Breakdown mechanisms.
- Ferroelectric materials: ferroelectric phase transition; domains; domain wall motion; hysteresis; case studies of BaTiO₃ and PZT.

Maxwell's equations

- Recap of Maxwell's equations & electromagnetic waves in 1D.
- Waves in free space, in insulating & conducting media polarisation of electromagnetic waves, impedance
- Waves in insulating & conducting media; the skin effect.

Optical Properties

- Reflection, refraction, absorption and propagation.
- Optic fibres: attenuation and intramodal dispersion
- Polarised light: birefringence; liquid crystal displays.

Further reading

Bleaney, B. I. and B. Bleaney. **Electricity and Magnetism**. Third edition, Oxford University Press, 2013. Oxford Classic Texts in the Physical Sciences.

Kittel, Charles and Paul McEuen. **Introduction to Solid State Physics**. Global edition, Wiley, 2018. Kittel's Introduction to Solid State Physics. Electronic Structure of Materials- Chapters 6, 7, 8. Magnetic Properties of Materials.

Moulson, A. J. and J. M. Herbert. **Electroceramics : Materials, Properties, Applications**. 2nd edition, Wiley, 2003. Dept. of Materials Library Overnight 44 MOU/1.

Solymar, L. and D. Walsh. **Electrical Properties of Materials**. 6th edition, Oxford University Press, 1998. Materials Dept. Library 21 SOL/Q.

General Paper 3: Mechanical Properties of Materials

General Paper 3: Mechanical Properties of Materials

Summary

This paper aims to develop a quantitative understanding of the mechanical properties of materials. Stress and strain are introduced as tensors, and both isotropic and anisotropic elasticity of materials are addressed, using worked examples that are relevant to fibre and particle composites, particle strengthening of metals and stress concentrations in engineering structures. Models to describe the relations between structure and elastic properties of composite materials and composite sheets are considered, then the elastic and viscoelastic behaviour of polymers is compared with the elastic behaviour of metals and ceramics. Plastic deformation and the brittle-ductile transition of polymers are addressed in the context of the glass transition. Plastic deformation in crystalline materials depends on the properties, motion and elastic interactions of dislocations, and these are considered in detail for both metals and non-metals, with an emphasis on the fundamental mechanisms of strengthening in metals through alloying and control of microstructure.

Plastic deformation, transformation of metastable phases and crazing in engineering materials gives them non-linear properties that can improve their resistance to cracks and strain concentrators. Using fracture mechanics, the key mechanisms of damage initiation in metals, ceramics, polymers and composites are addressed, including fatigue and the detrimental effects of environment. The design of composite materials to control their failure strength is also discussed, including long fibre, short fibre and particulate reinforcement. High temperatures impose very demanding conditions on materials. The design of resistant materials requires a detailed understanding of the mechanisms of creep and the influence of microstructure. With emphasis on metals and ceramics, the prediction and control of creep failure and practical applications of creep are discussed.

Mechanical Properties of Materials comprises three sections

- Elastic Deformation of Materials (10 lectures)
- Plastic Deformation of Materials (10 lectures)
- Structural Failure of Materials (16 lectures)

Elastic Deformation of Materials

Overview

This course builds on the introductory material from Prelims, particularly on Elastic Deformation and Mechanical Properties. A tensor-based mathematical approach is taken allowing consideration of both isotropic and anisotropic situations. Some topics (e.g. stress/strain relationships, Mohr's circle, yield criteria, plastic instability and rules of mixtures) are revisited in this tensor framework in order to reinforce key concepts and demonstrate their application in more complex situations. Continuum elasticity and macroplasticity can generally be applied to all types of homogeneous material and at all length scales. However, some important aspects that are particular to polymers and composites are also considered.

Elasticity theory (5 lectures)

- Mechanisms of elastic deformation in materials (revision)
- Definitions of strain and stress
- Strain as a deformation field.
- Coordinate transformations of strain tensors, Mohr's circle for strain.
- Stress and Hooke's law
- Strain and stress problems
- Hydrostatic stress, pressure and strain
- Equilibrium equations for stress, tensor transformation and Mohr's circle for stress and strain
- Compatibility equations for strain.
- Plane stress and plane strain. Airy stress function.
- Elasticity in cylindrical and spherical polars.
- General description of anisotropic elasticity (tensor notation).
- Worked examples on stress and strain

- Cylindrical symmetry: Misfitting fibre in an elastic medium.
- Spherical symmetry: Misfitting particle in an elastic medium.
- Interaction between a dislocation and a misfitting particle.
- Constraints of strain energy and symmetry on anisotropy – the reduced compliance matrix.

Elastic Properties of Composites (2 lectures)

Elastic stiffening in composites due to fibres and particles

- Rules of mixtures: Voigt and Reuss (revision). Halpin-Tsai.
- Elastic shear lag model for short fibres (results only, not full derivation), stress transfer length, efficiency factor.

Elastic behaviour of composite sheets

- Orthotropic plates, reduced compliance tensor, stress and strain transforms.
- Off axis properties, compliance transforms.

Deformation of Polymers (3 lectures)

Mechanisms of polymer deformation

- Elastic deformation and Glassy behaviour.
- Rubbery behaviour.
- The glass transition temperature.
- Yielding (and necking) in polymers

Rubber elasticity in polymers

- Entropic effects.
- Applications of rubbers/elastomers.

Linear viscoelasticity of polymers

- Creep and Stress relaxation. Spring and dashpot models (revision).
- The standard linear solid. Boltzmann and Time-temperature superposition.

Essential reading

Hull, Derek and T. W. Clyne. **An Introduction to Composite Materials**. Second edition, Cambridge University Press, 1996. Cambridge Solid State Science Series. Online. "Introduction to composite materials For Elastic Properties of Composites lectures".

McCrum, N. G. et al. **Principles of Polymer Engineering**. 2nd edition, Oxford University Press, 1997. Dept. of Materials Library 45 McM/3C. For Elastic Properties of Composites lectures

Ward, I. M. and J. Sweeney. **An Introduction to the Mechanical Properties of Solid Polymers**. 2nd edition, Wiley, 2004. Dept. of Materials Library 45 WAR/4A. For Elastic Properties of Composites lectures

Further reading

Advani, Suresh G. and Kuang-Ting Hsiao. **Manufacturing Techniques for Polymer Matrix Composites (Pmcs)**. Woodhead Pub., 2012. Woodhead Publishing in Materials. Online. Polymer matrix composites For Elastic Properties of Composites lectures

Bansal, Narottam P. and Jacques Lamon. **Ceramic Matrix Composites: Materials, Modeling and Technology**. The American Ceramic Society: Wiley, 2015. Ebook Central. Dept. of Materials Library 44 BAN. For Elastic Properties of Composites lectures

Billmeyer, Fred W. **Textbook of Polymer Science**. 3rd edition, Wiley, 1984. Dept. of Materials Library Overnight 45 BIL/B. Rheology and the Mechanical Properties of Polymers. For Elastic Properties of Composites lectures

Cottrell, Alan. **The Mechanical Properties of Matter**. Wiley, 1964. Wiley Series on the Science and Technology of Materials. Dept. of Materials Library 50 COT/2C.

Davim, J. Paulo and Igor S. Batraev. **Metal Matrix Composites: Materials, Manufacturing and Engineering**. De Gruyter, 2014. Ebook Central. Online. Metal matrix composites For Elastic Properties of Composites lectures

Dieter, George E. **Mechanical Metallurgy**. 3rd edition, McGraw-Hill, 1986. McGraw-Hill Series in Materials Science and Engineering. Chapter 2.

Gupta, Manoj. **Metal Matrix Composites**. MDPI - Multidisciplinary Digital Publishing Institute, 2018. online. Metal matrix composites For Elastic Properties of Composites lectures

Kumar, Anil and Rakesh K. Gupta. **Fundamentals of Polymer Engineering**. Third edition, CRC Press, 2019. For Elastic Properties of Composites lectures

Robinson, P, author et al. **Failure Mechanisms in Polymer Matrix Composites**. 1st edition, Woodhead Publishing, 2012. Online. Polymer matrix composites For Elastic Properties of Composites lectures.

Rudin, Alfred and Phillip Choi. **The Elements of Polymer Science and Engineering**. Third edition edition, Elsevier/AP, 2013. Online.

Sadd, Martin H. **Elasticity: Theory, Applications, and Numerics**. Third edition, Elsevier, 2014. Ebook Central. Online.

Sperling, L. H. **Introduction to Physical Polymer Science**. 4th edition, Wiley, 2006. Online Resource. For Elastic Properties of Composites lectures

Timoshenko, Stephen and J. N. Goodier. **Theory of Elasticity**. 3rd edition, McGraw-Hill, 1970. Engineering Societies Monographs. Dept. of Materials Library.

Vasiliev, Valery et al. **Advanced Mechanics of Composite Materials**. 2nd edition, Elsevier Science, 2007. Ebook Central. Online. *Elasticity of composites For Elastic Properties of Composites lectures

Further advanced reading

Gay, Daniel et al. **Composite Materials: Design and Applications**. CRC Press, 2003. *More advanced. For Elastic Properties of Composites lectures

Plastic Deformation of Materials

Overview

The properties, motion and elastic interactions of dislocations in crystalline materials are considered in detail for metals and non-metals. There is an emphasis on the fundamental mechanisms of strengthening in metals, through alloying and control of microstructure. This is illustrated with examples of important metallurgical case studies (aluminium-copper alloys and steels, in preparation for more detailed study in subsequent lecture courses).

Dislocations (6 lectures)

Introduction: Mechanisms of plastic deformation in materials (revision)

- Dislocations in ceramics and metals
- Plastic deformation mechanisms in polymers
- Plastic deformation mechanisms in glasses

Geometry of dislocations (revision)

- Burgers vector, Burgers circuit (FSRH convention).
- Edge, screw and mixed dislocations. Dislocation nodes and loops.

Elastic properties of dislocations

- Stress fields around dislocations, strain energy and total energy of dislocations.
- Forces on dislocations. Forces between dislocations. Stable arrangements of dislocations.
- Dislocations and free surfaces (Image forces). Dislocation line tension.

Dislocation motion and strength of crystalline solids

- Dislocation sources and multiplication, cross-slip.
- Plastic strain due to dislocation movement.
- Peierls energy and Peierls stress (lattice resistance). Thermally activated glide. Kinks, jogs and climb.

Dislocations in cubic close-packed metals

- Perfect dislocations, Shockley partial dislocations and intrinsic stacking faults.
- The Thompson tetrahedron. Lomer-Cottrell locks. Cross-slip. Frank partial dislocations.
- Ordered intermetallics: superdislocations, antiphase boundaries and the yield stress anomaly (Example: gamma prime precipitates in Ni-superalloys).

Dislocations in hexagonal close-packed metals

- Basal and non-basal slip.

Dislocations in body-centred cubic metals

- Core structures of screw and edge dislocations. Effects on glide and cross-slip.

Dislocations in non-metals

- Ionic and covalent crystals.

Strengthening Mechanisms in Metals (4 lectures)

Intrinsic strength and solid solution effects

- Bonding type and Peierls stress (revision).
- Temperature and strain rate.
- Solid solution size effect. Interaction with dislocations.
- Cottrell atmospheres, yield point phenomena, other solute interactions.

Flow Stress

- Effects on mobile dislocations of random arrays of obstacles (weak, strong, localised and diffuse).
- Solid solution strengthening: solute concentration.
- Precipitates and particles: coherent, semi-coherent and incoherent.
- Example: heat treatment of aluminium.

Microstructural effects

- Grain boundaries and phase boundaries.
- Hall-Petch relation; dislocation pile-up.
- Example: heat treatment of steel (non-examinable).

Texture

- Macro texture, micro texture, fibre and sheet textures.

Work hardening

- Strain hardening in single and polycrystals.
- Recovery mechanisms and recrystallisation (revision).
- Work hardening and plastic instability (revision).

Ideal microstructures for strength.

Essential reading

Hull, Derek and D. J. Bacon. **Introduction to Dislocations**. 5th edition, Elsevier Butterworth-Heinemann, 2011. Dept. of Materials Library 54 HUL/1. Chapters 1 to 8, Chapter 4 (section 4.5), Chapter 9 (section 9.1), Chapter 10 (sections 10.1 to 10.9)

Further reading

Cahn, R.W and P Haasen. **Physical Metallurgy**. 4th edition, Elsevier Science, 1996. Ebook Central. Online. A useful background text.

Hertzberg, Richard W. et al. **Deformation and Fracture Mechanics of Engineering Materials**. Fifth edition edition, John Wiley & Sons, Inc., 2013. Dept. of Materials Library Overnight 54 HER/G. Chapter 3 (Controlling Strength) - sections 3.1 to 3.8). Earlier editions (in print) are equally good but may have different chapter numbering.

Martin, J. W. **Worked Examples in the Strength of Metals and Alloys**. Institution of Metallurgists, 1983. Monograph (Institution of Metallurgists (Great Britain)) ; No. 11. Dept. of Materials Library 53 MAR/2B. Not online, but a useful read.

Porter, David A. et al. **Phase Transformations in Metals and Alloys**. 3rd ed. edition, CRC ; Taylor & Francis [distributor], 2009. Dept. of Materials Library 53 POR/I. Chapter 5, section 5.5, (Precipitation in Age-hardening Alloys). Earlier editions (in print) are equally good.

Structural Failure of Materials

Overview

Linear elastic fracture mechanics of brittle materials and the typical features in fracture of metals, polymers, composites was introduced in year 1. This course of lectures extends this to the failure of engineering materials, which can have non-linear properties and may accommodate the effects of cracks and strain concentrators by plastic deformation, transformation of metastable phases and crazing. The lectures consider first the fracture of materials due to static or rising loads, and then lifetime of materials with emphasis on fatigue due to cyclic loading and creep failure due to static loads at high temperature. The key mechanisms of damage initiation in the microstructures of metals, ceramics, polymers and composites are described. The design of composite materials to control their failure strength is discussed, including case studies of long fibre, short fibre and particulate reinforcement. There is a detailed consideration of the mechanisms of creep and the influence of microstructure, principally in metals and with comparison to ceramics also. Creep failure and practical applications of creep are discussed, including methods to predict creep life and improve creep resistance through control of microstructure. Finally, the engineering assessment of fatigue life is introduced, and mechanisms of fatigue and fatigue life estimation are considered, including the detrimental effects of environment and treatments that can be used to improve the fatigue resistance of metallic materials and structural components.

Fracture of Materials (8 lectures)

Background and revision

- Ideal strengths of materials in tension. Real strengths of materials. Brittle fracture.
- Griffith relation: Generalising Griffith, Mechanical energy release rate, G.

Linear Elastic Fracture mechanics

- K , K_{IC} . Toughness measurement in brittle materials.

Crack tip plasticity and inelastic deformation

- Irwin model for plastic zone: Plastic constraint, Plane strain toughness testing.
- Elastic-Plastic Fracture Mechanics: crack opening displacement (COD), J -Integral, Ductile-brittle transition (DBT) in fracture testing.
- Inelastic deformation. Examples: transformation of metastable phases and crazing in ceramics and polymer crazing/rubber toughening)

Initiation of fracture in metals and ceramics

- Nucleation, growth and coalescence of ductile cavities at particles.
- Surface damage in brittle materials. Intergranular fracture.
- Weibull Statistics

Mechanisms of brittle/ductile transitions

- Metals: Cleavage and the brittle/ductile transition, Influence of particle dispersions.
- Polymers: mechanisms of the brittle/ductile transition

Strength of composite materials

- Rule of mixtures for strength
- Longitudinal, transverse & shear strength of long fibre composites
- Longitudinal strength of short fibre composites
- Strength of particulate composites

Fracture of composite materials

- Failure mechanisms in composites (revision)
- Toughening mechanisms (examples)
- Work of fracture for fibre pull-out
- Examples: carbon fibre/epoxy for aerospace; silicon carbide/silicon carbide composites for aerospace/nuclear; tungsten carbide cutting tools, lightweight metal matrix composites

Lifetime Prediction of Materials (8 lectures)

Introduction to Creep

- Time dependent deformation, creep curves, Andrade's law, regions of creep, importance of creep.

Creep mechanisms in metals and ceramics

- Dorn equation, Orowan equation, Stress-directed diffusion.

Creep by movement of lattice dislocations

- Harper-Dorn creep
- Power-law creep: work hardening versus recovery, Bailey-Orowan equation, pipe diffusion, power law breakdown

Diffusion creep

- Herring-Nabarro creep, Coble creep, Grain boundary sliding.

Deformation mechanism maps

- Creep map examples in metals and ceramics
- Constant grain size, constant temperature.

Creep failure

- Cavity nucleation and cavity growth (diffusional growth, plastic growth) in metals
- Creep life prediction: Monkman-Grant, Larson-Miller parameter.

Optimisation of creep life

Case Studies:

- Nickel-based superalloys: polycrystalline vs monocrystalline.
- Superplastically, emphasising titanium alloys
- Ice

Fatigue of Materials

- Definitions; mechanical and microstructural characteristics
- S-N curves: fatigue limit and endurance limit, high and low cycle fatigue, Basquin, Coffin-Manson.
- Goodman and Miner descriptions of fatigue life.

Stages of fatigue in metals

- Mechanisms of crack initiation and crack growth.
- Stress intensity factor range and the Paris law; use in life predictions. Threshold stress intensity factor range.

- Short cracks.
- Effect of environment and metallurgical variables on fatigue life.
- Treatments to improve fatigue life.
- Strategies to design against fatigue failure:
 - Life-to-first-crack
 - Damage tolerant approaches
 - Concept of redundant design

Further Reading

Anderson, T. L. **Fracture Mechanics: Fundamentals and Applications**. 3rd edition, CRC/Taylor & Francis, 2005. Dept. of Materials Library 54 AND.

Derby, B. et al. **Materials for Engineering: A Fundamental Design Approach**. Longman Scientific & Technical, 1992. Chapter 8.

Dieter, George E. **Mechanical Metallurgy**. 3rd edition, McGraw-Hill, 1986. McGraw-Hill Series in Materials Science and Engineering.

Ewalds, H. L. and R. J. H. Wanhill. **Fracture Mechanics**. Edward Arnold, 1984. Dept. of Materials Library 54 EWA/D.

Green, D. J. **An Introduction to the Mechanical Properties of Ceramics**. Cambridge University Press, 1998. Cambridge Solid State Science Series. esp. Chapter 8.

Hertzberg, Richard W. **Deformation and Fracture Mechanics of Engineering Materials**. 3rd ed., International student edition, Wiley, 1989. Dept. of Materials Library 54 HER/D.

Honeycombe, R. W. K. **The Plastic Deformation of Metals**. Edward Arnold, 1968. Dept. of Materials Library 54 HON/D. esp. Chapters 7,13-15

Knott, J. F. and P. A. Withey. **Fracture Mechanics: Worked Examples**. 2nd ed; 1998 ed.cloM Communications Ltd. reprinted with corrections edition, Institute of Materials, 1993. Book (Institute of Metals); No. 550. Dept. of Materials Library 54 KNO/3A.

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

Hull, Derek and T. W. Clyne. **An Introduction to Composite Materials**. Second edition, Cambridge University Press, 1996. Cambridge Solid State Science Series. Online.

Knott, J. F. **Fundamentals of Fracture Mechanics**. Butterworths, 1973. Dept. of Materials Library 54 KNO/D.

Suresh, S. **Fatigue of Materials**. Second edition, Cambridge University Press, 1998. Dept. of Materials Library 54 SUR/B.

Martin, J. W. **Micromechanisms in Particle-Hardened Alloys**. Cambridge University Press, 1980. Cambridge Solid State Science Series. Dept. of Materials Library 54 MAR/2A. esp. Chapter 3

Matthews, F. L. and R. D. Rawlings. **Composite Materials: Engineering and Science**. Chapman & Hall, 1994.

Nabarro, F. R. N. and H. L. De Villiers. **The Physics of Creep: Creep and Creep-Resistant Alloys**. Taylor & Francis, 1995. Dept. of Materials Library Overnight 54 NAB/1.

Pelleg, Joshua. **Creep in Ceramics**. Springer, 2017. Solid Mechanics and Its Applications; V. 241.

Poirier, Jean-Paul. **Creep of Crystals: High-Temperature Deformation Processes in Metals, Ceramics and Minerals**. Cambridge University Press, 1985. Cambridge Earth Science Series. Dept. of Materials Library 30 POI/A.

Reed, Roger C. **The Superalloys: Fundamentals and Applications**. Cambridge University Press, 2006. Dept. of Materials Library 52 REE.

Ward, I. M. and D. W. Hadley. **An Introduction to the Mechanical Properties of Solid Polymers**. Wiley, 1994. Dept. of Materials Library 45 WAR/3.

Ward, I. M. and J. Sweeney. **An Introduction to the Mechanical Properties of Solid Polymers**. 2nd edition, Wiley, 2004. Dept. of Materials Library 45 WAR/4A.

Young, Robert J. and P. A. Lovell. **Introduction to Polymers**. 3rd edition, CRC Press, 2011.

General Paper 4: Structure and Thermodynamics of Materials

General Paper 4: Structure and Thermodynamics of Materials

Summary

This paper covers topics related to the structure and thermodynamics of materials and how to characterize them. It begins with an introduction to statistical mechanics to bridge from the quantum world of atoms to macroscopic quantities in thermodynamics, paying particular attention to thermal properties of materials. The observed properties of materials are closely linked to their composition, and microstructure, so it is essential that the right characterisation techniques are used and their limitations understood. The second lecture course in this paper will provide with a comprehensive review of some of the most widely used characterisation techniques nowadays. The third course will describe what we have learnt from years and years of materials characterisation in the areas of phase transformation.

Structure and Thermodynamics of Materials comprises:

- Statistical Mechanics and Thermal Properties of Materials (8 lectures)
- Characterisation of Materials (16 lectures)
- Phase Transformations (16 lectures)

Common themes in these topics are the use of quantum mechanical principles to underpin thermal properties and many of the measurement techniques applied to materials characterisation, and the link between statistical mechanics and thermodynamics which influences phase transformations of materials.

Statistical Mechanics and Thermal Properties of Materials

Overview

This course builds on the introduction to quantum theory and statistical physics in the first year to show how these ideas can be developed to understand the thermal properties of materials. It begins with a recap of extracting statistical predictions from quantum theory. It then builds up the theory of statistical mechanics and formalises the links to classical thermodynamics. It describes how to use these ideas to derive materials properties including heat capacities, paramagnetic susceptibility, and concentration of Schottky defects in a crystal.

Systems of free particles are then considered. The Bose-Einstein and Fermi-Dirac distribution functions are derived for bosonic and fermionic particles. The heat capacity of a free electron gas is covered. The concept of phonons as waves in a crystal is introduced, leading to the Debye model for specific heat capacities and the understanding of thermal conductivity in solids.

Recap of statistics in quantum mechanics

- Eigenstates and eigenvalues
- Calculating probabilities of measurement outcomes
- Expectation values
- Statistical variances and uncertainty

Introduction to statistical mechanics

- Microstates and macrostates, equal probability of microstates, the microcanonical ensemble as a model to describe statistical behaviour.
- Entropy related to number of microstates ($S = k \ln W$) and second law of thermodynamics. Application to ideal gas.
- Stirling's approximation
- Temperature in the microcanonical ensemble

Thermal equilibrium and the Boltzmann distribution

- Paramagnetic spin lattice – heat capacity and magnetic susceptibility
- Schottky defects
- The canonical ensemble describing systems at thermal equilibrium
- The partition function Z and Boltzmann's distribution.
- Application of Z to the paramagnetic spin lattice

The Einstein model of specific heat

- The quantum harmonic oscillator
- Partition function for a harmonic oscillator
- Einstein model of specific heat. Quantum and classical limits.

The bridge to thermodynamics

- Entropy in the canonical ensemble
- The Helmholtz free energy $F = -kT \ln Z$ and use to calculate materials properties.
- Application to gases and solids
- Anharmonic vibrations in crystals. The coefficient of thermal expansion and the Grüneisen parameter.

Statistics of Fermions and Bosons

- Distribution functions for identical particles – Bose-Einstein and Fermi Dirac
- k -space and the density of states for particles in a box
- Introduction to the free electron model, the Fermi energy and the heat capacity of metals

Lattice vibrations in solids

- Phonons as waves in a crystal
- Phonon dispersions and Brillouin zones
- The Debye model of specific heat

Thermal conductivity

- Heat conduction by free electrons
- Heat conduction by phonons
- Temperature dependence of thermal conductivity

Further Reading

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

Blundell, Stephen and Katherine M. Blundell. **Concepts in Thermal Physics**. 2nd edition, Oxford University Press, 2010. Dept. of Materials Library 22 BLU/1.

Bowley, Roger and Mariana Sánchez. **Introductory Statistical Mechanics**. 2nd edition, Clarendon, 1999. Dept. of Materials Library Overnight 20 BOW.

Chapters 1-10

Glazer, A. M. and J. S. Wark. **Statistical Mechanics: A Survival Guide**. Oxford University Press, 2001. Chapters 1-8

Hook, J. R. and H. E. Hall. **Solid State Physics**. 2nd edition, Wiley, 1991.

Manchester Physics Series. online. Chapters 2 and 3

Kittel, Charles and Paul McEuen. **Introduction to Solid State Physics**. 8th edition, Wiley, 2005. Dept. of Materials Library Overnight 22 KIT/1N. Chapters 4, 5 and 6.

Structural and Compositional Characterisation of Materials

Overview

This course of lectures will introduce the basics of the most commonly used techniques for the characterisation of materials, including microstructure and chemistry. Key concepts such as magnification, resolution and detectability limits will be explained, together with the operation and design of state-of-the-art instrumentation. An understanding of the fundamental mechanisms underpinning each instrument will provide an ability to critically judge the advantages and disadvantages of the different techniques and hence the ability to design an optimum characterisation strategy to address real-life materials problems. The course covers both Structural Characterisation (imaging and diffraction) and the Compositional Characterisation (FTIR, Raman, EDX etc, SIMS, APT), although these boundaries are not absolute. The course will be illustrated by examples and case studies demonstrating the implementation of characterisation techniques in further understanding the development of materials microstructure.

Introduction to characterisation techniques

- Microstructural and analytical characterisation
- Magnification and resolution
- Detectability limits

Introduction to Optical microscopy

- Anatomy of a microscope: Illumination system, apertures and lenses
- Illumination and imaging modes (including Kohler illumination, phase contrast, dark field and polarization)
- Diffraction, resolution and contrast
- Introduction to Raman and FTIR

Introduction to Electron Microscopy

- Electron generation and interaction with matter (revision)
- SEM (Scanning Electron Microscopy)
- EBSD (Electron Backscatter Diffraction) and TKD (Transmission Kikuchi diffraction)
- TEM (Transmission Electron Microscopy) and STEM (Scanning Transmission Electron Microscopy)
- Different imaging modes, definition of resolution, examples of instrumentation

Analytical Characterisation in Electron Microscopy

- Intro to EDX (Energy Dispersive X-ray) and EELS (Electron Energy Loss Spectroscopy) analysis (including instrumentation, basic spectral features and limitations)
- Intro to WDS (Wavelength-Dispersive Spectroscopy), Auger Spectroscopy and XPS (X-ray Photoelectric (including instrumentation, basic spectral features and limitations)
- Qualitative analysis
- Quantitative analysis (including cross-sections, background subtraction, curve fitting and errors)

Introduction to X-ray Characterisation Techniques

- X-ray generation and interaction with matter
- Laboratory Based vs Synchrotron X-ray characterisation
- Case study: WAXS characterisation of polymer crystallinity
- XRD (X-ray Diffraction), including powder diffraction
- XAS (X-ray absorption spectroscopy)
- Micro-CT (Computed X-ray Tomography)
- SAXS (Small Angle X-ray Scattering)

Introduction to Scanning Probe Techniques

- STM (Scanning Tunnelling Microscopy)
- AFM (Atomic Force Microscopy)

Introduction to Mass Spectrometry Techniques

- Creating ions: Ionization, desorption and sputtering
- FIB (Focused Ion Beam)
- Mass selection: Time-of-flight, quadrupoles and sector field

- SIMS (Secondary-Ion Mass Spectrometry)
- APT (Atom-probe tomography), including origins of the technique from FIM (Field Ion Microscopy)

Further reading

Cullity, B. D. and Stuart R. Stock. **Elements of X-Ray Diffraction**. 3rd edition, New international edition, Pearson Education, 2001. Dept. of Materials Library 31 CUL/J

Gault, Baptiste. **Atom Probe Microscopy**. Springer, 2012. Springer Series in Materials Science, 160. Dept. of Materials Library 32 GAU.

Goldstein, Joseph. **Scanning Electron Microscopy and X-Ray Microanalysis**. Third edition, Springer, 2003.

Goodhew, Peter J. et al. **Electron Microscopy and Analysis**. 3rd edition, Taylor & Francis, 2000. Dept. of Materials Library 32 GOO/B.

Lifshin, Eric. **X-Ray Characterization of Materials**. Wiley-VCH, 1999.

Murphy, Douglas B. and Michael W. Davidson. **Fundamentals of Light Microscopy and Electronic Imaging**. 2nd edition, Wiley-Blackwell, 2012. Ebook Central. Online.

Sanderson, J. B. **Understanding Light Microscopy**. 1st edition, John Wiley & Sons, Inc., 2019. Rms - Royal Microscopical Society.

Van der Heide, Paul. **Secondary Ion Mass Spectrometry: An Introduction to Principles and Practices**. Wiley, 2014. Ebook Central.

Voigtländer, Bert. **Scanning Probe Microscopy : Atomic Force Microscopy and Scanning Tunneling Microscopy**. Springer, 2015. Nanoscience and Technology.

Williams, David B. and C. Barry Carter. **Transmission Electron Microscopy: A Textbook for Materials Science**. 2nd. ed. [One-vol. edition, Springer, 2009. Dept. of Materials Library 32 WIL/4A.

Phase Transformations

Overview

The aim of this course is to teach the fundamentals of phase transformations and how they apply to different classes of materials, including metals, ceramics and polymers. After an introduction to the balance between the thermodynamic driving force and the kinetics (rate) of a phase transformation, the course covers underpinning concepts necessary for the rest of the course: diffusion, ternary systems, and surface and interface structure, thermodynamics and mobility. Then we will cover the key stages of a phase transformation; nucleation, growth and then the laws that describe the rates of phase transformations. This is then contrasted with 'diffusionless' phase transformations like ordering. Examples from real engineering materials are included throughout.

Introduction

- Kinetics vs thermodynamics: role of interface energy.
- Progress of a reaction and the classification of transformations.

Diffusion

- Mechanisms of migration in various materials types.
- Solutions to Fick's Law: annealing times, thin layers, multilayers.
- Diffusion in substitutional alloys
- Diffusion and chemical potentials

Ternary phase diagrams

- Gibbs triangle, isothermal sections, contour maps. Lever rule. Free energy curves.
- Three phase reactions.
- Four phase reactions. Ternary eutectic. Quasi Peritectic. Ternary peritectic.
- Examples of engineering ternary diagrams.

Surfaces, Interfacial structure and Mobility

- Thermodynamic degrees of freedom and excess quantities at interfaces
- Measurements of surface and interfacial energy
- Gibbs-Duhem equation; Thermal grooving; Triple junctions and wetting; Interfacial segregation.
- Gibbs-Thompson effect and Ostwald ripening
- Characterisation, anisotropy and shape of precipitates.
- Anisotropy of surface and interfacial energy
- Facetting, coherency, and the Jackson alpha factor model of S/L interfaces.
- Continuous and step growth mechanisms in S/L interfaces.
- Solid state interface mobility, glissile interfaces.
- Martensitic (martensitic) transformations

Nucleation

- Homogeneous and heterogeneous nucleation.
- Nucleation in the solid state: incubation, strain effects, transition phases and coherency loss.

Alloy solidification

- Solute distributions, including the Scheil equation.
- Constitutional supercooling and interface stability.
- Macro- and micro-segregation in castings.

Crystallisation of polymers

Growth of precipitates; diffusion and interface control

Grain growth

Phase transformations in Al-alloys

Other important processes

- Widmanstätten precipitation
- Spinodal decomposition

Rate laws and Avrami equation

- Interface-controlled vs diffusion-controlled growth.
- Rate laws for different growth geometries and coarsening.
- The Avrami equation and growth exponents for different situations.

Coupled growth mechanisms

- Eutectic/eutectoid and cellular transformations.

'Diffusionless' transformations

- Ordering, recrystallization and the massive transformation

Further reading

Abbaschian, R. et al. **Physical Metallurgy Principles**. 4th edition, SI edition, Cengage Learning, 2010. Dept. of Materials Library 50 REE/H.

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.

Askeland, Donald R. et al. **The Science and Engineering of Materials**. Seventh edition. SI edition edition, Cengage Learning, 2016. Dept. of Materials Library Overnight 50 ASK/1.

Cottrell, Alan. **An Introduction to Metallurgy**. 2nd edition, Institute of Materials, 1995. Book (Institute of Materials (Great Britain)); 626. Dept. of Materials Library 50 COT/3.

Porter, David A. and K. E. Easterling. **Phase Transformations in Metals and Alloys**. 2nd edition, Chapman & Hall, 1992. Dept. of Materials Library 53 POR/H.

Smallman, R. E. and A. H. W. Ngan. **Modern Physical Metallurgy**. Eighth edition, Butterworth-Heinemann, 2014. Ebook Central. Dept. of Materials Library 50 SMA.

Other Lectures

Maths - Partial Differential Equations & Fourier Series and Tensors

Overview

The technique of Fourier Series, and the related method of Fourier Transforms (which will be touched on in the course) provide a powerful and intuitive method for tackling real-world problems: By breaking up a complex scenario into a simple description in terms of sine and cosine functions, we can solve differential equations for heat and vibration problems that have realistic boundary (e.g. starting) conditions. The course is quite visual with the lecturer using maths software to show what is happening; students may like to use maths tools on a laptop to follow along.

Many materials are anisotropic, which can mean that the constant of proportionality between, for example, a cause vector (e.g. electric field) and the effect vector (electric current) is different in different directions. This lecture course sets up the mathematical foundations for describing such behaviour and relates it to the different crystal systems. Various tensors are considered such electrical and thermal conductivity and thermal expansion and the tensor treatment of optical properties is also considered. Tensor properties are also important in elasticity and micro-plasticity of materials. The lecturer will make use of mathematics software for illustrating and visualising most important concepts.

Fourier Series

Background revision on the nature of periodic functions.

Introducing the notion of composing a general period function from a sum of elementary functions; Fourier's theorem.

Special cases of Fourier series; examples including the square and triangular waves.

Exploring Fourier Series with MATLAB.

Fourier series for functions with periods other than 2π . Integration and differentiation of Fourier series.

Approximating periodic functions by finite sums of trigonometric functions.

Complex form of Fourier series.

Introduction to the Fourier Transform

Fourier transforms as a generalisation of Fourier series.

Applications of Fourier transforms, and exploration with MATLAB.

Partial differential equations

Revision of core concepts for differential equations.

Diffusion equation

- Derivation of the diffusion equation.
- Solution of the diffusion equation for
 - Simplified initial condition (sinusoidal distribution of density)
 - Realising initial conditions (block-like initial distribution)

The latter introducing the notion of ***separation of variables***.

Introduction to the problem of a semi-infinite volume;

- Derivation of the complementary error function by similarity transformation.

Wave equation for a taut string

- Derivation of the wave equation; static and travelling waves.
- Analysing the frequency composition of a plucked string.

Tensors

Basic principles

- Scalar and vector variables
- Tensor properties
- Crystal symmetry, Neumann's principle
- Transformation of vectors and tensors
- Representation surface, principal axes

Second-rank tensors

- Electrical and thermal and conductivity
- Stress and strain
- Thermal expansion
- Electrical and magnetic susceptibility
- Optical properties of crystals

Essential reading

Lovett, D. R. **Tensor Properties of Crystals**. Hilger, 1989. Dept. of Materials Library 30 LOV. Chapter 1-6. Looks a bit old fashioned but covers everything you will need.

Nye, J. F. **Physical Properties of Crystals: Their Representation by Tensors and Matrices**. Clarendon Press, 1998. Oxford Science Publications.

Further reading

Bolton, W. **Fourier Series**. Longman Scientific & Technical, 1995. Mathematics for Engineers ; No. 4. Dept. of Materials Library Overnight 1 0 BOL. A gentle introduction to Fourier series. There is a copy in the RSL, and St Edmund Hall has one in its library. This book doesn't cover all the topics in the lecture course, however.

Brown, James Ward and Ruel V. Churchill. **Fourier Series and Boundary Value Problems**. 8th edition, McGraw-Hill, 2012. Brown and Churchill Series.

comprehensive book. We'll mainly be concerned with the material in the first four chapters.

Chandrasekhar, S. **Liquid Crystals**. 2nd edition, Cambridge University Press, 1992. Dept. of Materials Library 30 CHA/A.

Feynman, Richard P. et al. **The Feynman Lectures on Physics**. Addison-Wesley, 1963. Materials Dept. Library 20 FEY/Bb or 20 FEY/Cc or 20 FEY/Ac. Volume II, Lecture 31

Gay, P. **An Introduction to Crystal Optics**. Longmans, 1967. Dept. of Materials Library 30 GAY.

Guinier, André. **The Structure of Matter: From the Blue Sky to Liquid Crystals**. Edward Arnold, 1984. Dept. of Materials Library Overnight 20 GUI.

Hartshorne, N. H. and A. Stuart. **Crystals and the Polarising Microscope**. 4th edition, Edward Arnold, 1970.

Hirth, John Price and Jens Lothe. **Theory of Dislocations**. McGraw-Hill, 1968. McGraw-Hill Series in Materials Science and Engineering. Dept. of Materials Library 54 HIR/B. Chapter 2.

Kelly, A. and Kevin M. Knowles. **Crystallography and Crystal Defects**. Third edition, John Wiley & Sons, 2020. 30 KEL and Electronic resource. Chapter 1-3. Good introductory chapters with a more contemporary feel.

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

Kreyszig, Erwin et al. **Advanced Engineering Mathematics**. 8th edition, Wiley, 1999. Dept. of Materials Library 1 0 KRE/D. Chapters 10 and 11 cover Fourier series and PDEs

MathWorks. www.mathworks.com. There are also excellent resources online, both for Fourier series / transformation, and for PDEs. Tutorials in MATLAB can also be found, on the www.mathworks.com site and elsewhere.

Riley, K. F. et al. **Mathematical Methods for Physics and Engineering**. 18th printing. edition, Cambridge University Press, 2019. Chapter 10 covers Fourier Series, and chapters 16 and 17 cover PDEs

Steeds, J. W. **Introduction to Anisotropic Elasticity Theory of Dislocations**. Clarendon Press, 1973. Monographs on the Physics and Chemistry of Materials. Dept. of Materials Library 54 STE.

Wood, Elizabeth A. **Crystals and Light: An Introduction to Optical Crystallography**. Published for the Commission on College Physics [by] Van Nostrand, 1964. Van Nostrand Momentum Books, No. 5. Dept. of Materials Library 30 WOO/3.

Wooster, W. A. **Tensors and Group Theory for the Physical Properties of Crystals**. Clarendon Press, 1973. Dept. of Materials Library 30 WOO.

Wooster, W. A. and A. Breton. **Experimental Crystal Physics**. 2nd edition, Clarendon Press, 1970. Dept. of Materials Library 30 WOO/2B.

Wooster, W. A. **A Text-Book on Crystal Physics**. Reprinted with corrections. edition, University Press, 1949.



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

