Materials Science (MS)
Prelims Lecture Course Synopses
2019-20

Department of Materials

Materials Science (MS)

Prelims Lecture Course Synopses 2019-20

Materials Science 1: Physical Foundations of Materials

Materials Science 1: Physical Foundations of Materials

Summary
This paper introduces the physical foundations underpinning important areas of Materials Science. You will learn some basic concepts of atomic arrangements in perfect crystals and how we can use diffraction of X-ray and electron waves to measure these arrangements. The use of waves will also be used to explore basic concepts in wave mechanics and quantum theory, and how these theories can be used to explore the behaviour of electrons in materials and how bonding occurs. Quantum theory involves randomness and probability, and these ideas are continued in the study of random processes in materials to explain phenomena such as diffusion and the behaviour of gases. The physical principles of electricity and magnetism are introduced and used to explore the electrical and magnetic properties that are so important for many applications of materials.

Comprises

- The Study of Crystalline materials by Diffraction (8 lectures)
- Electromagnetic Properties and Devices (12 Lectures)
- Random Process and Statistical Physics (8 Lectures)
- Wave mechanics, Quantum Theory and Bonding (12 Lectures)

MS1: Physical Foundations of Materials — Michaelmas Term

1st year MS

Prof A.I. Kirkland

8 lectures

The Study of Crystalline Materials by Diffraction

Overview

The vast majority of materials are crystalline, and so any study of materials must start with introducing some basics of crystallography including the use of a unit cell to describe the periodicity in the crystal and how to represent symmetry in crystals. In a crystal, the atoms form a periodic lattice that can act as a diffraction grating to radiation, and diffraction is therefore an important characterisation tool. The use of diffraction as a practical tool for identifying crystal structures in materials will be introduced.

Lecture Content

Lecture 1. The Periodic lattice

Definitions of a lattice, mesh, unit mesh and motif

The Unit Cell and basis vectors

The structure of metals and some binary compounds

Lecture 2. Symmetry in 2D

Symmetry elements in 2D

Lattice symmetry in 2D

The 2D plane point groups

Lecture 3. Crystallographic planes and directions

Miller and Miller Bravais indices describing planes and directions

Calculation of interplanar spacings, angles between planes and directions

Lecture 4. Waves

Wave particle duality for X-Rays, electrons and neutrons

Mathematical representation of harmonic travelling waves

Interference of waves and the principle of superposition

Lecture 5. Diffraction in 2D and 3D

Diffraction from a 2D grating, the effects of slit width, separation and grating size

Diffraction from a 3D lattice; The Laue equation

Braggs law

Lecture 6. Scattering by atoms

Scattering factors for electrons, X-rays and neutrons

Structure factors

Forbidden reflections in cubic systems

Lecture 7. The reciprocal lattice

Constructing the reciprocal lattice

The Ewald sphere construction for single crystal and powder diffraction

Observing the reciprocal lattice with electron diffraction

Lecture 8.

Practical X-ray, electron and neutron diffraction experiments

Indexing powder x-ray and electron diffraction patterns

Example phase identification using powder diffraction

Recommended text books

Hammond: **The basics of crystallography and diffraction**

Kelly, Groves and Kidd: **Crystallography and Crystal Defects**

MS1: Physical Foundations of Materials Hilary Term

1st year MS

Prof S.C. Speller

12 lectures

Electromagnetic Properties and Devices

Overview

Next generation batteries for electric vehicles; sustainable materials for touch screen displays; faster, more compact and efficient computing; futuristic cloaking devices: these are just a few examples of the wide range of technological applications which exploit electromagnetic phenomena in materials. This course introduces the physics of classical electromagnetism and how different kinds of material respond to electrical and magnetic fields. We will explore how the structure of a material influences its electromagnetic properties including the origins of phenomena such as ferroelectricity and piezoelectricity, and how the coupling between electric/magnetic/strain fields can be exploited in real devices.

Part I: Electrical properties of materials

Theory of electrostatics

- Basic concepts of charge, force on a charge, potential and electric field, capacitance
- Calculations using superposition principle and Gauss' theorem in examples with simple geometries

Dielectric materials

- Concepts of polarisation, dielectric permittivity, susceptibility, and electric displacement (D).
- Calculations involving simple geometries of capacitor.
- Example devices

Piezoelectric, pyroelectric and ferroelectric materials

- Concept of coupling between fields (e.g. electrical and strain)
- Crystal symmetry requirements
- Examples of materials
- Applications (e.g. Atomic Force Microscope, ferroelectric RAM)

Electrical transport

- Basic concepts of current, current density, resistance, Ohm's law.
- Electrical conductivity of metals – Drude model
- DC circuits

Part II: Magnetic properties of materials

Theory of magnetostatics

- Concepts of magnetic field, flux and induction.
- Calculations of magnetic field from currents in simple geometries using Biot-Savart and Ampere's laws (e.g. straight wire, loop, solenoid, toroid)
- Lorentz force on charges moving in electric fields

Electromagnetic induction

- Faraday's law and Lenz's law
- Concepts of self and mutual inductance

Magnetic materials

- Concepts of magnetisation, magnetic susceptibility, magnetic permeability and magnetic intensity (H)
- Introduction to paramagnetic, diamagnetic and ferromagnetic materials
- Applications of ferromagnets (saturation magnetisation, hysteresis loops, remanent field, coercivity, hard and soft ferromagnets)
- Example magnetic devices

Part III: Electromagnetic waves

General theory of electromagnetism

- Maxwell's equations in integral form
- Concept of displacement current

Electromagnetic waves

- General wave equation
- Formulation in integral form

Interaction of materials with EM waves

- Refractive index
- Conductors
- Example applications

Top

Recommended text books

W J Duffin, **Electricity and Magnetism**, McGraw-Hill. Good basic text with similar level of mathematical complexity as lecture course.

Bleaney & Bleaney, **Electricity and Magnetism**, OUP. More advanced text - rather old fashioned

Solymar, & Walsh, **Electrical Properties of Materials**, Oxford University Press. More advanced text - interesting examples

Background reading

Feynman, **Lectures on Physics**, Addison-Wesley, Vol II, Ch. 1-22 are worth reading. The mathematical formalism is more complex, but is clearly explained in the text. Vol. 1, Ch. 2 gives an interesting historical overview of "Basic Physics" which helps set the classical physics discussed in this course in context.

MS1: Physical Foundations of Materials Hilary Term

1st year MS

Prof R.S. Weatherup

8 lectures

Random Processes and Statistical Physics

Overview

Quantum theory shows us that probability plays an important role in the processes that control materials properties. This course explores that idea in more detail, looking at how randomness can control structure, how it plays a role in diffusion processes and in the interaction of gases with surfaces. The statistical concepts introduced can be used to explain classical thermodynamics, and the statistical natures of heat capacity is introduced.

Lecture Content

Random processes in materials

Examples of random processes e.g. diffusion

Random walks – applications (e.g. polymers)

Rapid random motion of gas molecules

Basic assumptions of kinetic theory

Simple derivations of pressure and temperature

Ideal gas equations

Statistical distributions of molecular motions

Statistical notation

Collision with walls – relating pressure to collision rate

Deposition of materials and thin film growth

Effusion

Pressure and distribution of velocities

Derivation of pressure as statistical average and need for mean-square velocity

Maxwell-Boltzmann distribution of velocities

Collisions and transport

Concept of mean free path

Rate of collisions in gases and relation to reaction kinetics (effect of temperature and pressure)

Rate laws. Determination of reaction order and rate constants/The Arrhenius equation.

Transport in materials – diffusion, heat flow and viscosity

Effect of temperature and pressure on transport

Molecular Dynamics – applications to liquid, diffusion in solids (non-examinable)

Non-ideal gas behaviour

Interaction between molecules

Modification to ideal gas law

Equipartition theory (links to thermodynamics course)

Heat capacity of gases

Breakdown of classical physics

Heat capacity of solids

Recommended Reading

Dill, K. A., & Bromberg, S. **Molecular Driving Forces: Statistical Thermodynamics in Biology, Chemistry, Physics, and Nanoscience**, Garland Science, Chapters 1-12, 17-19

Seddon, J. M., Gale, J. D., **Thermodynamics and Statistical Mechanics**, The Royal Society of Chemistry, Chapter 8-11,13

Atkins, P., de Paula, J., & Keeler, J. **Atkin's Physical Chemistry**, Oxford University Press, Focus 1

Background Reading

Kittel, C. & Kroemer, H., **Thermal Physics**, W. H. Freeman and Company

MS1: Physical Foundations of Materials Hilary & Trinity Terms

1st year MS

Dr R.J. Nicholls & Prof P.D. Nellist

12 Lectures

Wave Mechanics, Quantum Theory and Bonding

Overview

Many properties of materials are controlled by how electrons behave in them. Because of wave-particle duality, we need to consider electrons as waves. This course shows how these ideas lead onto quantum theory and the idea of discrete states. We can then think about what happens over different length scales including atoms and nanomaterials. The concept of bonding and molecular orbitals is introduced before thinking about entire crystals and how bands are formed.

Lecture Content

Wave particle duality

Evidence, electron diffraction, photoelectric effect, atomic spectra

DeBroglie wavelength

Interpretation of quantum mechanical wave

Observation of quantum systems

Perturbation of observed systems

Postulates of quantum mechanics

Operators and commutators

Uncertainty principles – momentum-space / energy-time

Waves and the wave equation

Wave packets

Dispersion, phase velocity and group velocity for electrons and photons

Schrödinger equation

Waves on a string, standing waves and boundary conditions

Mathematical notations for waves

Free and fixed boundaries

Nodes and antinodes

Harmonics

Wave equations

Infinite potential well

Infinite potential well

Waves in a 1D box, quantisation, quantum confinement

Illustrated with energy levels in nanomaterials (QDs etc.)

Measurement in quantum mechanics

Decomposition into eigenstates

Statistical nature of measurements and expectation values

Wavefunction collapse and Schrödinger's cat

Transmission and reflection of waves

Finite boundary potentials

Boundary condition matching

Transmission and reflection coefficients

Tunnelling and evanescent waves

Extension to 3D

Separation of variables

Angular momentum

Quantum numbers *n* and *l*

The hydrogen atom

One electron atoms

Heavier atoms

Spin

Fermions and bosons

Pauli exclusion principle

Filling of atoms

Multiple finite wells

Molecular orbital theory – bonding and antibonding

The concept of the broadening of discrete states into bands

The concept of a crystal momentum to describe a wave

Recommended text books

Phillips, **Introduction to Quantum Mechanics**, Pitched at a similar level to the course

Blinder, **Introduction to Quantum Mechanics in Chemistry**, Materials Science and Biology, Goes a bit faster than Philipps, but also has a lot of background about further applications in science

Griffiths, **Introduction to Quantum Mechanics**, More formal and mathematical and goes a bit deeper

Background Reading

Gasiorowicz, **Quantum Physics**, A classic text book in the field

Materials Science 2: Structure and Mechanical Properties of Materials

Top

Materials Science 2: Structure and Mechanical Properties of Materials

Summary

This paper introduces the basic structures of materials –both crystalline and amorphous and how they deform and fail under applied stresses. You will learn the theory behind methods used to study the atomic arrangement in perfect crystals and in then apply these to the common lattice defects which can occur. How these defects control the mechanical properties of the materials will be introduced in both single crystal and more engineering relevant material systems. This will cover elastic properties, including stress and strain analysis, yield phenomenon, post yield plastic flow and linear elastic fracture mechanics.

Comprises

- Elastic Deformation (8 lectures)
- Structures of Crystalline and Glassy Materials (12 lectures)
- Defects in Crystals (8 lectures)
- Mechanical Properties (12 lectures)

MS2: Structure and Mechanical Properties of Materials Michaelmas Term

1st year MS

Prof A. J. Wilkinson

8 Lectures

Elastic Deformation

Overview

This course introduces the basics of stress and strain. Analysis of simple bending conditions (cantilever, three point, four point) as required for mechanical testing analysis are developed, including shear force and bending moment diagrams. Mohr's circle is introduced as a graphical method to calculate stress or strain states at any point in a plane for arbitrary loading conditions. The underlying physics of elastic constants and how they relate stress and strain will be derived. Time dependant elastic deformation (viscoelasticty) will be introduced through examples in polymeric materials. Stress states and the elastic deformation of thin wall pressure vessels and torsional deformation of prismatic rods will be discussed.

Lecture Content

Equilibrium

Resolving forces

Taking moments

Internal forces

Shear force and bending moment diagrams

Stress

Definitions, normal stress, shear stress, notation

Transformation of axes

Resolving stress onto an inclined plane

Mohr's circle for stress

Principal stresses, maximum shear stress

Strain

Definitions, normal strains, shear strain

Engineering and tensor strains

Transformation of axes

Mohr's circle for strain

Principal strains, maximum shear strain

Elasticity and interatomic forces

Recap of fundamentals

Physical basis for Hooke's law

Hooke's law

Relating stress and strain

Young's Modulus

Shear modulus, bulk modulus

Poisson's ratio

Viscoelastic deformation

Simple spring and dash pot models

Elastic deformation examples

Thin wall pressure vessels

Bending of beams

Torsional deformation

Recommended Reading

Dieter, G. E., **Mechanical Metallurgy**, McGraw-Hill, Chapter 2

Benham, P.P., Crawford, R. J., Armstrong C. G., **Mechanics of Engineering Materials**, Harlow: Longman

Gere, J. M., & Goodno, B. J., **Mechanics of Materials**, Cengage Learning

McCrum, N. G., Buckley. C. P., & Bucknall, C. B., **Principles of Polymer Engineering**, Oxford University Press, Chapter 4

MS2: Structure and Mechanical Properties of Materials Michaelmas & Hilary Terms

1st year MS

Prof K.A.Q. O'Reilly & Prof M. L. Galano

12 Lectures

Structures of Crystalline and Glassy Materials

Overview

This course will investigate why different classes of materials exist and how different forms of interatomic bonds lead to different materials properties. Ways to represent and describe bonding will be introduced through the use of example materials with common crystal structures. Key classes of materials (ceramics, metals, polymers, glasses) will be introduced and specific applications of these materials used to illustrate key points.

Lecture Content

Types of Bonding

Examples of simple crystal structures

Close packing of spheres. FCC and HCP and stacking sequences

Octahedral and tetrahedral interstices in close-packed structures

Basic Concepts

- Definition of metals, ceramics, polymers, glasses and semiconductors
- Types of bonding: ionic, covalent, metallic, van der Waals
- Dependence of interatomic forces on distance
- Non-directional bonds: van der Waals, metallic; close packing
- Directional bonds: the covalent bond, hybrids
- Electronegativity, ionic bonding, co-ordination
- Trends in the periodic table

Stereographic projections and the Weiss zone law

Pole figures

Stereographic projection. Properties of projection

Great circles, Small circles, Zones

Preservation of angular truth

Wulff net

Zone axes, Zone symbols

Weiss zone law

Crystallographic calculations

Addition rule, Use in plotting stereogram

Use to illustrate coordination, e.g. for tetrahedral structures, and symmetry directions in common lattice, e.g. cubic

Examples from real structures (e.g. zinc blende, wurtzite, NiAs)

Ceramic materials bonding

Ionic Structures

- Structures of composition AX (CsCl, NaCl, ZnS)
- Principles of ionic bonding: radius ratio criterion, energy considerations, Madelung constant
- Structures of composition AX2
- Pauling's Rules

Covalent Structures

- Simple covalent structures (diamond, graphite)
- Molecular crystals
- Structures of some ceramics.

Perovskite structures

- Basic properties

Glasses and amorphous materials

Idea of local ordering

SiO_2 coordination

Network formers

Basic properties of glasses

Bonding and structure of polymers, molecular crystals, polymorphism

Mixtures of bonding. Tg. Random walk model

Thermosetting vs thermoplastics v rubbers

- Rubber, polyethene, nylon6-6

Polymer properties

- Degree of polymerisation
- Molecular weight distribution
- Stereoregularity

Glass transitions

Metals, solid solutions and ordered alloys

Trends across the Periodic Table

Typical metallic structures (FCC, BCC, HCP); atomic packing factor, unit cell volume, theoretical density

Relationship between structure, bonding and properties of pure metals

Interstitial and substitutional alloys – iron-carbon, iron-chromium, aluminium-copper

Hume-Rothery Rules: size factor, electrochemical factor & relative valency factor

Electron compounds; normal valency compounds; size factor compounds - interstitial compounds

Recommended Reading

Cottrell, **An Introduction to Metallurgy,** Inst. of Materials, 50COT/3

Moffatt, Pearsall & Wulff, **The Structure and Properties of Materials**, Wiley, chapter 1-3, 50WUL/Ba

Evans, **An Introduction to Crystal Chemistry**, CUP,

Hume Rothery & Haworth, **The Structure of Metals and Alloys**, Parts II to V, Hume Rothery, 50HUM/2

Kittel, C., **Introduction to Solid State Physics**, Wiley, chapters 1 & 3, 22KIT

Hammond, C., **The Basics of Crystallography and Diffraction**, IVC/OUP, 30HAM

Kelly, A. & Knowles, K., **Crystallography & Crystal Defects**, Wiley, 30KEL

Callister, W. D. & Rethwisch D. G., **Materials Science and Engineering**, Wiley, 50CAL

Phillips, F. C., **An Introduction to Crystallography**, Oliver & Boyd, 30PHI

Background Reading

Kelly, A. & Groves, G. W., **Crystallography and Crystal Defects**, Longman, 30KEL

Smallman, **Modern Physical Metallurgy**, Butterworth- Heinemann, 50SMA

Sperling, L. H., **Introduction to Physical Polymer Science**, Wiley-Interscience , reference book

Barratt, C. S. & Massalski, T. B., **Structure of Metals**, Pergamon, 31BAR/1H

MS2: Structure and Mechanical Properties of Materials Hilary Term

1st year MS

Dr P. Chen

8 lectures

Defects in Crystals

Overview

This course will introduce the basic forms of defects present in crystalline materials. Their effect on physical properties will be considered. Diffusion of point defects and implications for systems such as ionic conductors will be covered. Dislocations will be given the fullest consideration. Differences between edge and screw dislocations. How dislocation move and control the mechanical properties in single crystal metals will be covered. Finally methods for imaging dislocations in the TEM and calculating their nature will be introduced. This course will build on the diffraction and crystal structures courses and also use elasticity analysis introduced in elasticity and structures. It will lead into the mechanical properties course.

Lecture Content

Introduction

Types of lattice defects (point, line, planar)

What do defects control – examples (semiconductors, strengthening in metals)

Point defects and diffusion

Concentration likelihood at different temperatures

Random walks

Concentration of point defects

Vacancy motion and solid state diffusion

Diffusion mechanisms and Fick's laws

Quirks of diffusion in ionic materials – diffusion on sublattices – relate to ionic conductors for Li batteries

Introduction to dislocations

Structure of edge and screw dislocations in simple cubic materials

Intrinsic and extrinsic properties

Definition of a Burgers vector

Dislocations in cubic lattices

Slip systems

Peach Koehler formula for force on dislocation

Dislocation sources

Motion of dislocations under applied stress

Dislocation motion in single crystals

Primary and secondary slip systems

Deformation of singles crystals in tension and compression

Self-energy of dislocations

Dissociation and partial dislocations

Introduction to stacking faults

Imaging dislocations

Etch pits methods

Introduction to diffraction contrast TEM imaging and grain boundary analysis

Planar defects

Introduction to grain boundaries, twins and antiphase boundaries

Structure of grain boundaries and concepts of grain boundary energy

Recommended Reading

Kelly, A. & Groves, G. W., **Crystallography and crystal defects**, London Longman

Reed-Hill, R. E. & Abbaschian, R., **Physical Metallurgy Principles**, CRC Press

MS2: Structure and Mechanical Properties of Materials   Trinity Term

1st year MS

Prof D. E. J. Armstrong

12 Lectures

Mechanical Properties

Overview

This course builds on the elastic behaviour course looking at how materials behave beyond the yield point and from the defects course, looking at how defects can control mechanical behaviour. The basic methods of materials testing will be introduced, this will link into several practical classes. Plastic behaviour will be covered both at the micro and macroscale. At the microscale building on the defects course, but concentrating on the strength of polycrystalline metals and introduce the concept of strengthening through precipitates, using aerospace aluminium alloys as examples. This will be followed by a macroscopic treatment of yield through Tresca, Von Mises and Coulombs Yield Criterion for deformation in bulk metals and polymers. Fracture will be covered in ceramics and glasses using a linear elastic treatment. Toughening mechanisms will be introduced including fibre toughening which will lead to a first treatment of composite materials. Finally optimisation of materials properties will be covered, looking at a range of properties including design for strength, stiffness and cost.

Lectures

Testing mechanical properties

Why we test, how we test, what we test.

Types of stress and strain

Introduction to stress- strain curves for metals, ceramics, polymers

Microscale mechanisms of plasticity and how we control plastic strength

Metals – chemistry and crystallographic effects

Metals –grain size; Hall-Petch effect, how to control grain size

Work hardening in metals. Single vs double slip. Effect of crystal structure and stacking fault energy on work hardening behaviour

Twinning deformation, difference to annealing twins

Plasticity in polymers, glass transitions temperatures

Predicting plastic failure at bulk or component length scales

Tresca and Von Mises yield criterion – metals

Coulomb yield criterion – polymers

Using yield criterion for combined tension-torsion loading

Fracture processes

Recap of theoretical strength

Stress concentrations at small flaws

Griffith theory

Orowan Modification

Ductile to brittle transitions in metals

Fracture and failure in polymers

Toughening mechanisms –transformation toughening, microcracking, composites

Introduction to mechanics of composites

Design of composites – examples from aerospace and F1

Rules of mixture in long fibre composites

Optimising materials selection

Ashby Maps

Examples of using Ashby Diagrams and properties optimisation (design for stiffness, lightness, strength, cost etc).

Reading list

There are many good books on mechanical properties. College, department and the Radcliffe Science libraries will all have a good selection, which will help you understanding. Below are some suggestions, but no single book will cover the whole course.

Recommended Reading

Callister & Rethwisch, **Materials Science and Engineering**,

Dieter, G. E., **Mechanical Metallurgy**, McGraw-Hill

Background Reading

Ashby & Jones, **Engineering Materials 1: An Introduction to Properties, Applications and Design**

Ashby**, Materials Selection in Mechanical Design**

The Dissemination of IT for the Promotion of Materials Science (DoITPoMS) website https://www.doitpoms.ac.uk/ has good introductions to many key concepts discussed in this course

Materials Science 3: Transforming Materials

Materials Science 3: Transforming Materials

Summary

This paper is introduces you to how the microstructure of materials can be transformed and controlled through processing, in order to control and optimise the properties that are required for the material to perform its function. The theory of thermodynamics is critical to all transformations in materials, and you will be introduced to the first and second laws of thermodynamics and their role in phase diagrams. This will be developed further in Microstructure and Processing of Materials I & II, which will describe how phase transformations can be used to control microstructure, with case studies in metallic, ceramic and polymeric systems. Electrochemical processes, which are driven by thermodynamics, are important in the production and degradation of materials, as well as the performance of materials for energy storage. The developing field of nanomaterials will then be introduced, with emphasis on nanomaterial synthesis, properties and applications.

Comprises

- Thermodynamics (8 lectures)
- Introduction to Nanomaterials (8 lectures)
- Microstructure and Processing of Materials I (8 lectures)
- Electrochemistry (8 Lectures)
- Microstructure and Processing of Materials II (8 lectures)

MS3: Transforming Materials — Michaelmas Term

1st year MS

Prof M.P. Moody

8 lectures

Thermodynamics

Overview

Thermodynamics is fundamental to the physical and chemical processes that occur in materials. This course underpins many subsequent parts of the materials degree. It focuses on the first and second laws of thermodynamic, using practical examples, and leads to an understanding of phase stability.

Lecture Content

First law of thermodynamics

Thermodynamic Definitions: work, heat, internal energy, state and path functions
Simple gas expansion
Reversible and irreversible processes

Enthalpy and heat capacity

Heat capacity at constant volume
Storage of internal energy
Constant pressure processes
Heat capacity at constant pressure
Enthalpy variation with temperature
Hess's law. Kirchhoff's equation

Entropy and the second law of thermodynamics

Definition of a spontaneous process
Entropy variation with temperature
Entropy of phase changes
Definition of the Gibbs function
Thermodynamic Master Equations
Gibbs function variation with temperature and pressure
Gibbs Helmholtz equation
Statistical mechanics definition of entropy

Mixtures and equilibria.

Dealing with mixtures

Chemical Potential

The Van't Hoff isochore

Applications of thermodynamics to metallurgy

Ellingham diagrams

Stability of oxides

Thermodynamics of the Blast Furnace

Extraction of metals from Sulphides

Predominance diagrams

Phase changes.

The phase rule and phase diagrams

The Clausius-Clapeyron equation

Vapour pressure. Ideal solutions

Non-ideal solutions

Free energy of mixing

Regular solutions

The quasi chemical model

Recommended Reading

Atkins and De Paula, **Physical Chemistry**

Part One Thermodynamics

1. *Properties of Gases*
2. *The First Law*
3. *The Second and Third Laws*
4. *Physical Transformations of Pure Substances*
5. *Simple Mixtures*
6. *Chemical Equilibrium*

(based on format of 10th Edition)

Gaskell, D. R. **Introduction to the Thermodynamics of Materials**

1. *Introduction And Definition Of Terms*
2. *The First Law Of Thermodynamics*

3. *The Second Law Of Thermodynamics*
4. *The Statistical Interpretation Of Entropy*
5. *Auxiliary Functions*
6. *Heat Capacity Enthalpy Entropy And The Third Law Of Thermodynamics*
7. *Phase Equilibrium In A One Component System*
8. *The Behavior Of Gases*
9. *The Behavior Of Solutions*
10. *Gibbs Free Energy Composition And Phase Diagrams Of Binary Systems*
11. *Reactions Involving Gases*
12. *Reactions Involving Pure Condensed Phases And A Gaseous Phase*

Background Reading

Atkins, **The Laws of Thermodynamics – A Very Short Introduction**

MS3: Transforming Materials Michaelmas Term

1st year MS

Prof N. Grobert

8 lectures

Introduction to Nanomaterials

Overview

This course serves as an introduction to the rapidly developing area of Nanomaterials, beginning with the peculiar characteristics of materials at the nanoscale and the new technologies they enable. Important methodologies for nanomaterial synthesis are described, and the structures of key nanomaterials are introduced, including carbon nanomaterials and chalcogenides. The upscaling of the manufacture of nanomaterials is considered, together with associated ethical and safety issues. The course concludes with current and potential applications of nanomaterials in medicine and energy.

Lecture Content

Introduction

Nanoscale,

Nanotechnology,

Surface areas per unit volume,

0-D, 1-D, 2-D materials

Synthesis of nanomaterials

Chemistry of particle synthesis,

Sol-gel processing,

Core-shell nanoparticles,

Composites, coatings, thin films,

Chemical vapour deposition, arc discharge, exfoliation

Carbon nanomaterials

Fullerenes, nanotubes, graphene

Other nanomaterials

Chalcogenides, other 2-deg materials

Manufacturing

Upscaling,

Safety of nanomaterials,

Ethics and regulation

Physical properties of nanomaterials

Introduction to electrical, optical and mechanical properties at the nanoscale

Applications of nanomaterials

Medical applications,

Energy materials

Recommended Reading

Di Ventra, **Introduction to Nanoscale Science and Technology**

Koch, **Nanostructured Materials: Processing, Properties and Applicatio**ns

Guldi and Martin, **Carbon nanotubes and related structures: synthesis, characterization, functionalization, and applications**

Karn, **Nanotechnology and the Environment**

Harris, P. F. J., **Carbon Nanotube Science, General Overview of CNTs**

Reich, S., Thomson, C., & Maultzsch, J., **Nanostructured Materials: Processing, Properties and Applications, Basic Concepts and Physical Properties of CNTs**

MS3: Transforming Materials Michaelmas Term

1st year MS

Prof C.R.M. Grovenor

8 lectures

Microstructure and Processing of Materials I

Overview

Material microstructures are the product of phase transformations that occur during their processing, so an understanding of phase transformations is important in all material systems. This course builds on the thermodynamics course to explain how phase diagrams are obtained, how they predict the equilibrium phases and reactions. These will be illustrated with examples of their use in the processing of metallic materials, including liquid-solid and solid-solid transformations.

Lecture Content

- Concepts of microstructure
- Terminology for microstructures
- Gibbs phase rule
- Solutions, compounds and mixtures
- Simple phase diagrams; tie lines and invariant points
- Ideal and regular solution models
- Tangent and lever rules

Phase diagrams

- Derivation from free energy-composition curves
- Continuous solutions, immiscibility and ordering
- Eutectic, peritectic, eutectoid peritectoid and monotectic reactions. Intermediate phases

Using phase diagrams

- Solidification: driving force for solidification; introduction to homogeneous and heterogeneous nucleation

- Solidification of solutions: partition coefficient; Scheil equation and segregation; cells and dendrites, cored microstructures.
- Eutectic and peritectic transformations and microstructures
- Solid state phase transformations:
- Introduction to precipitation homogeneous and heterogeneous nucleation; : Equilibrium precipitation and age hardening
- Heat treatments:
- Introduction to recrystallization and grain growth

Background Reading

Porter, Easterling, **Phase transformations in metals and alloys**,

Cottrell, A. H., **An introduction to metallurgy**,

Smallman, Ngan, **Modern Physical Metallurgy**, Elsevier

https://downloadfiles.grantadesign.com/pdf/booklets/Teach_Yourself_Phase_Diagrams_and_Phase_Transformations.pdf,

Askeland, **The Science and Engineering of Materials**, Chapman Hall

MS3: Transforming Materials Hilary Term

1st year MS

Prof M. Pasta

8 lectures

Electrochemistry

Overview

Electrochemistry is fundamental to the extraction of metals by electrolysis and also their corrosion and protection from degradation. The same processes of electrochemical thermodynamics are critical to the design and performance of materials for electrochemical energy storage, and sensors that rely on electrochemical processes. This course provides an introduction to applications of electrochemistry, and considers the thermodynamics of electrochemical processes. Factors that influence the kinetics of electrochemical reactions, including transport properties and interfaces are considered, using case studies.

Lecture Content

Introduction to electrochemistry

Overview: electrodes, electrolytes and interfaces

Applications:

- Electrolysis
- Electrodeposition and electroplating
- Electro-mining
- Electroanalysis and sensors
- Corrosion and protection
- Energy conversion, production and storage

Electrochemical thermodynamics

The physics of phase potentials

Cell potential and Gibbs free energy

Electrochemical potential

Half-reactions and standard reduction potentials

Cell potential and concentrations: Nernst equation

Reference electrodes

Pourbaix Diagrams

Case studies: sensors (potentiometry), maximum theoretical specific energy in batteries

Electrolytes and transport properties

Electroneutrality

Non-ideal behaviour of electrolyte solutions: activity coefficient

Transport properties: conduction, diffusion, migration

Case studies: activity coefficient, diffusion coefficient and transference number

The electrode-electrolyte interface: the electrical double layer

Structure of the electrical double layer

Case study: supercapacitors

Kinetics of electrode reactions

Charge transfer across the interface

Overpotential

Butler-Volmer model and the Tafel equation

Case study: electrocatalysis

Recommended Reading

Bard, Allan, **Electrochemical Methods: Fundamentals and Applications**, Wiley

Background Reading

Jiri Koryta, Jiri Dvorak, Ladislav Kavan, **Principles of Electrochemistry**, Wiley

1st year MS

Prof C.R.M. Grovenor

8 lectures

Microstructure and Processing of Materials II
(Draft)

Overview

These lectures build on the preceding course, using case studies in metallic (solidification and heat treatment), polymeric and ceramic systems, to develop an understanding of how the microstructures of materials can be controlled through processing.

Lecture Content

Casting and Al-Si

- Ingot solidification and cooling curves
- Structures of cast metal, facetting, Na modification
- Engineering applications

The Fe-C system

- Eutectic reaction and cast irons
- Eutectoid decomposition
- Hypo and hyper eutectoid alloys
- Martensite and bainite
- TTT curves. Typical microstructures for different heat treatments
- Engineering applications

Polymers:

- Polymer blends and crystallisation
- Manufacturing techniques
- Engineering applications

Ceramics:

- Powder processing
- Sintering

- Ceramic microstructures
- Engineering applications

Reading list *tbc*

Porter & Easterling: **Phase Transformations in Metals and Alloys**

Cottrell, **An introduction to Metallurgy**

Ashby and Jones, **Engineering Materials 2**

Askeland, **The Science and Engineering of Materials**

Mathematics for Material Science

Mathematics for Material Science

Summary

Mathematics is the language of the physical sciences. This course will cover the mathematics which will underpin the material science you will learn this year, and in future years. As well as learning the fundamentals you will gain experience at applying mathematics to physical problems.

Comprises:

Mathematics for Materials Science I

- Ordinary and Partial Differentiation (7 Lectures)
- Vectors & Matrices (12 lectures)

Mathematics for Materials Science II

- Taylor Series and Limits (3 lectures)
- Integration (5 lectures)
- Complex Numbers (4 lectures)
- Ordinary Differential Equations (6 lectures)

Recommended Reading

Stephenson, G. **Mathematic Methods for Science Students**, Longman Mathematical
Riley, K. F., Hobson, M. P., Bence, S. J. **Methods for Physics and Engineering**
Boas, M.K., **Mathematical Methods in the Physical Sciences**

1st year MS

Dr E. Liberti

Prof S.C. Benjamin

19 lectures

Mathematics for Material Science I

Ordinary and partial differentiation (EL)

Differentiation from 1st principles, chain rule

Partial Differentiation (EL)

Total derivatives, exact differentials,

Change of variables, chain rule

Applications: Spherical and polar coordinates, thermodynamics

Vectors (SCB)

Scalar Product and Vector Product.

Introduction to Vector Calculus

Applications: Reciprocal lattice, Miller indices and planes

Matrices (SCB)

Inverse matrices

Determinants

Orthogonal matrices

Properties of symmetric Matrices - eigenvalues and eigenvectors

Applications: Conductivity – interpretation of principle value and directions.

Mathematics for Material Science II — Hilary Term

1st year MS

Dr A.W. Robertson

Dr N. Ares

18 lectures

Mathematics for Material Science II

Integration (AWR)

Evaluation of definite integrals by substitution, partial fractions, integration by parts and reduction formulae

Multiple integrals in two and three dimensions - including polar and spherical coordinates.

Applications: areas, volumes, centroids, bending moments, Random Processes and Statistical Physics

Complex numbers (AWR)

Exponential form.

Argand Diagrams

de Moivre's theorem

Solutions of Polynomial Equations.

Applications: Complex Impedance, circuits involving inductors, capacitors and resistors.

Taylor series and limits (NA)

Taylor series, limits and l'Hopital's rule

Applications: Low and high temperature expansions

Ordinary differential equations (NA)

First Order equations: Separable variables. Linear homogeneous equations – integrating factor as a method of solution.

Applications: Cooling, circuits

Second Order Equations: Linear homogeneous with constant coefficients. Linear homogeneous with constant coefficients. Method of solution via auxiliary equation and particular integral.

Applications: Resonance in electrical and mechanical systems.

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