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

Prelims Lecture Course Synopses 2019-20
<table>
<thead>
<tr>
<th>Course Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Materials Science 1: Physical Foundations of Materials</td>
<td>3</td>
</tr>
<tr>
<td>The Study of Crystalline Materials by Diffraction</td>
<td>5</td>
</tr>
<tr>
<td>Electromagnetic Properties and Devices</td>
<td>7</td>
</tr>
<tr>
<td>Random Processes and Statistical Physics</td>
<td>10</td>
</tr>
<tr>
<td>Wave Mechanics, Quantum Theory and Bonding</td>
<td>12</td>
</tr>
<tr>
<td>Materials Science 2: Structure and Mechanical Properties of Materials</td>
<td>15</td>
</tr>
<tr>
<td>Elastic Deformation</td>
<td>17</td>
</tr>
<tr>
<td>Structures of Crystalline and Glassy Materials</td>
<td>19</td>
</tr>
<tr>
<td>Defects in Crystals</td>
<td>22</td>
</tr>
<tr>
<td>Mechanical Properties</td>
<td>24</td>
</tr>
<tr>
<td>Materials Science 3: Transforming Materials</td>
<td>27</td>
</tr>
<tr>
<td>Thermodynamics</td>
<td>29</td>
</tr>
<tr>
<td>Introduction to Nanomaterials</td>
<td>32</td>
</tr>
<tr>
<td>Microstructure and Processing of Materials I</td>
<td>34</td>
</tr>
<tr>
<td>Electrochemistry</td>
<td>36</td>
</tr>
<tr>
<td>Microstructure and Processing of Materials II</td>
<td>38</td>
</tr>
<tr>
<td>Mathematics for Material Science</td>
<td>40</td>
</tr>
<tr>
<td>Mathematics for Material Science I</td>
<td>42</td>
</tr>
<tr>
<td>Mathematics for Material Science II</td>
<td>43</td>
</tr>
</tbody>
</table>
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)
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
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
    o Basic concepts of charge, force on a charge, potential and electric field, capacitance
    o Calculations using superposition principle and Gauss’ theorem in examples with simple geometries
  Dielectric materials
    o Concepts of polarisation, dielectric permittivity, susceptibility, and electric displacement (D).
    o Calculations involving simple geometries of capacitor.
    o Example devices
  Piezoelectric, pyroelectric and ferroelectric materials
    o Concept of coupling between fields (e.g. electrical and strain)
    o Crystal symmetry requirements
    o Examples of materials
    o Applications (e.g. Atomic Force Microscope, ferroelectric RAM)
Electrical transport
  o Basic concepts of current, current density, resistance, Ohm’s law.
  o Electrical conductivity of metals – Drude model
  o DC circuits

Part II: Magnetic properties of materials

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

Electromagnetic induction
  o Faraday’s law and Lenz’s law
  o Concepts of self and mutual inductance

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

Part III: Electromagnetic waves

General theory of electromagnetism
  o Maxwell’s equations in integral form
  o Concept of displacement current

Electromagnetic waves
  o General wave equation
  o Formulation in integral form

Interaction of materials with EM waves
  o Refractive index
  o Conductors
  o Example applications
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.
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
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
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)
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 (viscoelasticity) 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**
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
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
Barratt, C. S. & Massalski, T. B., Structure of Metals, Pergamon, 31BAR/1H
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
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**

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/](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)
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
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 Applications
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
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
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**

**Background Reading**
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
1st year MS

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

Mathematics for Materials Science II
  o Taylor Series and Limits (3 lectures)
  o Integration (5 lectures)
  o Complex Numbers (4 lectures)
  o Ordinary Differential Equations (6 lectures)

Recommended Reading

Stephenson, G. Mathematical 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
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

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)
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.