MSc in Materials Science

Module specifications

School of Mathematics and Physics
Queen's University Belfast

PHYxx11 Fundamentals of Materials Science

Level and credits
Level M; 30 CATS.

Pre-requisites / Co-requisites
None.

Module content
The module will introduce students to the fundamentals of materials science. The starting point for much of materials science is how materials are held together by different types of bonds in different crystal structures. These atomic arrangements affect many different macroscopic properties of materials. Specific topics include:

- Bonding in materials
    - Ionic
    - Covalent
    - Molecular
    - Metallic
- Crystallography including crystal defects
- Anisotropy
- Thermal properties
- Mechanical properties
- Phase diagrams and microstructure
- Materials classes
    - Metals
    - Polymers
    - Ceramics

Learning outcomes
On completion of this module, the successful student will be able to

- Critically describe and discuss different types of bonding and their effect on materials properties.
- Critically describe and discuss different types of crystal structure and their influence on materials properties.
- Critically describe and discuss how microstructure is developed in engineering materials and its effect on materials properties.
- Define and identify the materials classes metals, polymers and ceramics and critically analyse in what applications they are useful.

Indicative time allocation

Structured study of course materials	60 hours
Electronic conferencing	60 hours
Assignments and quizzes	60 hours
Independent learning time	120 hours

Assessment

Assignments	20%	On-line participation	15%
In course tests	15%	End-of-module examination	50%

Supplementary notes

PHYxx12 Materials Characterisation

Level and credits
Level M; 20 CATS.

Pre-requisites / Co-requisites
None

Module content
This compulsory module introduces the fundaments for some of the most widely used characterisation techniques used to examine materials. The techniques are varied, from those techniques used for imaging, compositional and structural information to those methods used to measure materials' properties. The following techniques will be covered:

- Spectroscopy: Infrared (IR) and Ultraviolet-Visible (UV-Vis).
- Other analytical techniques.
- X-ray Diffraction.
- Scanning Probe Microscopy (SPM).
- Electron Microscopy.

Learning outcomes
At the end of this module the student will have achieved the following learning outcomes:

- Deep understanding of the basic principles behind each characterisation technique.
- Be able to critically review and critique the practical aspects of each technique.
- Critically evaluate the use one or more methods for a particular case.

Indicative time allocation

Structured study of course materials	40 hours
Electronic conferencing	40 hours
Assignments and quizzes	40 hours
Independent learning time	80 hours

Assessment

Assignments	20%	On-line participation	15%
In course tests	15%	End-of-module examination	50%

Supplementary notes

PHYxx13 Materials Science Case Study

Level and credits
Level M; 10 CATS.

Pre-requisites / Co-requisites
Fundamentals of Materials Science and Materials Characterisation

Module content
The aim of this module is to bring together the skills and knowledge gained in the Fundamentals of Materials Science and Materials Characterisation applying them to a real engineering materials science case. As such this module will present the students with a problem in material engineering, that they will suggest solutions to using a variety of materials characterisation techniques and their knowledge of materials properties.

Learning outcomes
On completion of this module, the successful student will be able to

- Critically discuss and select appropriate materials characterisations techniques for a specific case.
- Independently plan a series of materials characterisation experiments or simulations and critically interpret the resulting data.
- Critically analyse and discuss how to choose a material for an engineering application and apply this to a specific case.

Course components

Problem-based learning	100 hours

Assessment

Oral or written report	60%
Continuous assessment	40%

Supplementary notes
There are two options for this module:

1. Residential case study, using the materials characterisation facilities in the School of Mathematics and Physics to obtain experimental data.
2. Distance learning case study, using simulated or theoretically obtained data, supplemented with experimental data provided by the module coordinator.

PHYxx21 Magnetic and Electronic Materials

Level and credits

Level M; 20 CATS.

Pre-requisites / Co-requisites

Fundamentals of Materials Science, Materials Characterisation, Materials Science Case Study

Module content

Magnetic materials are currently used in a range of applications including data storage, engines and sensors. This module covers magnetic properties of materials from the atomic origin of magnetic dipole moments to magnetic engineering materials. Specific topics include:

- Atomic dipole moments
- Diamagnetism
- Paramagnetism
- Ordered magnetic materials
    - Ferromagnetism
    - Antiferromagnetism
    - Ferrimagnetism
    - Other ordered magnetic materials
- Magnetic materials characterisation techniques
- Applications of magnetic materials

For millennia, human technology has predominantly valued the physical properties of materials, such as strength, hardness and toughness. In recent decades, however, this situation has completely changed. It is now the manner in which a material interacts with an electric field that most often determines its technological usefulness. Developing an understanding of the ways in which different material groups behave under electric bias is the focus of the electronic materials part of this module. Specific topics include:

- Transport in Electronic Materials:
    - Free electrons and metals.
    - Thermally excited carriers and semiconductors.
    - Lattice-carrier coupling: polarons and superconductors.
    - Ionic conductors and their applications.
    - Characterisation of carriers (use of Hall and Seebeck effects, Impedance Spectroscopy).
    - 2D conduction (LAO/STO, graphene and planar domain walls); diagnostics of confined transport (e.g. quantum Hall effect).
- Non-Conducting Systems
    - Dielectrics and ferroelectrics.
    - Multiferroics and magnetoelectric coupling.
- Metal-Insulator Phase Transitions.

Learning outcomes

On completion of this module, the successful student will have achieved the following learning outcomes:

- Deep understanding of the fundamental physics of magnetic properties of materials.
- Be able to critically describe and discuss different types of magnetic behaviour in materials.

- Familiarity with magnetic characterisation techniques including ability to critically discuss data interpretation and limitations.
- Be able to correctly categorize the magnetic properties needed for an application and critically discuss and suggest appropriate materials.
- Deep understanding of the fundamental physics of materials responsible for differing kinds of response under electric fields.
- Familiarity with a significant number of specific electronic material types, including the ability to critically discuss their similarities and differences.
- Be able to correctly categorize the electronic properties needed for an application and critically discuss and suggest appropriate materials.

Indicative time allocation

Structured study of course materials	40 hours
Electronic conferencing	40 hours
Assignments and quizzes	40 hours
Independent learning time	80 hours

Assessment

Assignments	20%	On-line participation	15%
In course tests	15%	End-of-module examination	50%

Supplementary notes

The module will be offered in a given year if a minimum of four students enrol on the module.

PHYxx22 Optical and Plasmonic materials

Level and credits

Level M; 20 CATS.

Pre-requisites / Co-requisites

Fundamentals of Materials Science, Materials Characterisation, Materials Science Case Study

Module content

This module will provide a comprehensive understanding of the optical and plasmonic properties of materials. This will include the introduction of the fundamental physical laws about light reflection and transmission, the optical properties of a broad range of materials, the structural colour in nature (such as the opalescence of butterfly wings, beetles and some plants), optical nonlinear effects of materials, and how to create exotic optical properties not seen in nature from artificial metamaterials (such as negative refraction materials). Topics covered include:

- The nature of light.
- Optical properties of dielectrics.
- Optical properties of metals.
- Optical properties of semiconductors.
- Optical properties of thin films.
- Optical properties of photonic crystals.
- Structural colour in nature.
- Optical nonlinear effects.
- Optical properties of metamaterials.

Plasmonics is a term used to describe physical phenomena connected with collective oscillations of the free electron gas in a solid. That means metals for the most part, but not exclusively. Thin film plasmonics had its experimental origin in the 1960s, but the field received major impetus with the emergence of nano-scale plasmonics in the late 1990s; today it is a burgeoning research area with applications beginning to grow. Various developments have come together to stimulate and sustain this field, notably advances in nano-fabrication techniques, the development of software packages for electromagnetic modelling and various innovations in optical and other microscopy techniques. The course will cover the fundamentals of plasmonics and plasmonic materials and metamaterials with due emphasis given to the fundamental physics, combined with description of (nano-)fabrication and optical analysis techniques. Application of plasmonic structures and materials in biosensing and other areas will also be addressed.

Topics covered in this module include:

- Dielectric properties of materials – what constitutes a plasmonic material.
- Bulk plasmons, surface plasmons and surface plasmon polaritons.
- Localised surface plasmons and metallic nanostructures.
- Optical and electronic excitation and detection of plasmons, including scanning probe microscopy techniques.
- Electromagnetic surface modes at low frequencies.
- Plasmon hybridisation in core-shell structures. Fano resonance in plasmonics.
- Optical antenna and plasmonic resonances; micro- and nano-scale antenna fabrication.

- Alternative plasmonic materials and plasmonic metamaterials.
- Fabrication of plasmonic structures and metamaterials.
- Field enhancement effects in plasmonics – surface enhanced spectroscopies and fluorescence.
- Recent trends in plasmonics – quantum plasmonics, non-locality, chiral plasmonics.
- Non-linear plasmonics – second harmonic generation and other non-linear effects.
- Applications of plasmons: biosensing, enhanced light generation and detection, heat assisted magnetic recording.

Learning outcomes

On completion of this module, a student will have achieved the following learning outcomes:

- Deep understanding of the basic optical properties of a range of materials
- Deep understanding what defines the optical properties of a material.
- Critical awareness of the importance of the structure of materials on their optical properties
- Deep understanding the origins of the structural colours of some insects and plants.
- Deep understanding the optical nonlinear effects of materials.
- Awareness of how to develop new materials for custom-designed optical properties and ability to critically discuss the process.
- Deep understanding of fundamental properties of propagating and localised surface plasmons.
- Ability to perform calculations on plasmon resonances and to critically analyse near-field and far-field optical data on plasmon excitation and detection.
- Deep understanding of the link between plasmon properties and design and implementation of plasmonic structures and materials e.g. thin film properties, optical antenna, dimer through to heptamer plasmonic structures, plasmonic metamaterials.
- Conduct an intelligent discourse on applications of plasmonics in areas such as spectroscopy, biosensing (and others) with reference to fundamental material properties and plasmon characteristics.

Indicative time allocation

Structured study of course materials	40 hours
Electronic conferencing	40 hours
Assignments and quizzes	40 hours
Independent learning time	80 hours

Assessment

Assignments	20%	On-line participation	15%
In course tests	15%	End-of-module examination	50%

Supplementary notes

The module will be offered in a given year if a minimum of four students enrol on the module.

PHYxx23 Electron Microscopy and Scanning Probe Microscopy

Level and credits

Level M; 20 CATS.

Pre-requisites / Co-requisites

Fundamentals of Materials Science, Materials Characterisation, Materials Science Case Study

Module content

This optional module develops from the Materials Characterisation module. The objective of this module is to provide a deeper understanding of the different imaging and analytical techniques in electron microscopy (EM) and scanning probe microscopy (SPM) to measure physical properties, as well as different specimen preparation methods. This module will cover both routine and latest developments of EM. The following techniques will be covered:

- Scanning electron microscopy.
- Transmission electron microscopy.
- Focused ion beam techniques.

This module will also cover practical and theoretical issues of advanced scanning probe microscopy (SPM) techniques ranging from fundamental physical studies to device characterisation, failure analysis, and nanofabrication. The technical aspects of SPM methods ranging from scanning tunnelling potentiometry to electrochemical SPM will be addressed along with the fundamental physical phenomena underlying the SPM imaging mechanisms. The latter half of the course will cover practical aspects of SPM characterization of a wide range of materials, including semiconductors, ferroelectrics, dielectrics, polymers, carbon nanotubes, and biomolecules, as well as SPM-based approaches to nanofabrication and nanolithography. Content will broadly include:

- Scanning probe microscopy techniques for electrical and electromechanical characterisation.
- Principles underlying a variety of scanning probe microscopy techniques, e.g. scanning tunnelling microscopy, scanning capacitance microscopy, piezoeresponse force microscopy .
- Electrical SPM characterization of materials and devices and nanofabrication techniques
- Theory of scanning probe microscopy.
- Applied aspects of SPM based functional characterisation of materials.

Learning outcomes

At the end of this module the student will have achieved the following learning outcomes:

- Be able to explain and critically discuss the principles of the different EM techniques.
- Deep understanding of the procedures for collecting and interpreting data (images).
- Breakdown and critically discuss the practical aspects of each technique, including sample specimen preparation.
- Assess and critically discuss the use of one or more methods for a particular case.
- Deep understanding of the different theoretical and practical aspects of SPM including the principles of operation behind different techniques.
- Identify and critically discuss the opportunities and limitations that each technique presents in the context of materials characterisation.

- Critically analyse practical situations of material characterisation and decide upon the relevant SPM techniques that could be applied in given scenarios for maximum functional information.
- Deep practical knowledge of SPM based techniques in specific aspects of characterisation of a wide range of material systems.

Indicative time allocation

Structured study of course materials	40 hours
Electronic conferencing	40 hours
Assignments and quizzes	40 hours
Independent learning time	80 hours

Assessment

Assignments	20%	On-line participation	15%
In course tests	15%	End-of-module examination	50%

Supplementary notes

The module will be offered in a given year if a minimum of four students enrol on the module.

PHYxx24 Thin Film Techniques and Sensor Technology

Level and credits

Level M; 20 CATS.

Pre-requisites / Co-requisites

Fundamentals of Materials Science, Materials Characterisation, Materials Science Case Study, Magnetic and Electronic Materials

Module content

Thin film deposition is widely used in much of today's high technology industry. For example it is required as a major part of all semiconductor based and data storage devices. The functionality required of the film can range from protecting against environmental attack to quantum tunnelling across a single atomic layer.

This module will cover various industrially relevant deposition techniques and the students will gain an appreciation for the properties of the thin films produced in each case. These properties will ultimately depend on the film microstructure and thickness and methods to evaluate these will be studied. Content covered includes:

- Deposition geometry.
- Physical vapour deposition.
- Chemical vapour deposition.
- Nucleation and growth.
- Microstructure.
- Thin film characterisation.
- Selected application examples.

This module will also introduce the student to a range of sensors widely used in materials science and engineering for both metrology and automation. The objective is to provide a framework to understand how sensors, transducers and devices interact with their environment and to understand some of the many practical considerations in the selection and implementation. The following topics will be covered:

- Basic principles of sensors and transducers such as type of sensor, linearity, hysteresis, sensitivity, threshold, cross-talk, resolution, dynamic range etc.
- Sources of noise and its measurement
- Active sensors such as photovoltaic, piezoelectric, thermoelectric, electromagnetic
- Passive sensors such as variable resistance and reactance
- The importance of micro-sensors and the emergence of nanoscale sensors such as magnetic sensors and biosensors

Learning outcomes

On completion of this module, the successful student will have achieved the following learning outcomes:

- An awareness of the range of deposition methods available for thin film growth and ability to critically discuss them.
- A deep understanding of how deposition conditions relate to film microstructure.
- A deep understanding of how to characterise thin films.

- An awareness of the range of applications that require control of thin film growth and ability to critically discuss them.
- Deep understanding of the critical factors used in the evaluation, selection and implementation of sensors.
- An awareness of the importance of different classes of materials in the creation and implementation of sensors and ability to critically discuss them.
- Be able to review and critique the suitability of different types of sensors for different sensing scenarios.

Indicative time allocation

Structured study of course materials	40 hours
Electronic conferencing	40 hours
Assignments and quizzes	40 hours
Independent learning time	80 hours

Assessment

Assignments	20%	On-line participation	15%
In course tests	15%	End-of-module examination	50%

Supplementary notes

The module will be offered in a given year if a minimum of four students enrol on the module.

PHYxx25 Materials modelling and simulation

Level and credits
Level M; 20 CATS.

Pre-requisites / Co-requisites
Fundamentals of Materials Science, Materials Characterisation, Materials Science Case Study

Due to the steady increase in computational power and the development of advanced simulation methods, computational modelling has become an almost indispensable tool in the analysis and development of new materials. This module will introduce students to a range of theoretical and computational techniques used in the modelling and simulation of materials. It starts by refreshing and consolidating the students' programming skills, then reviews the important concepts in classical, quantum and statistical mechanics. The core topics of the module are: electronic structure calculations, development of force fields, and simulation methods in statistical mechanics. There will be a significant hands-on component consisting of developing simple simulation and analysis codes, and training in the use of electronic structure and molecular simulation packages.

Specific topics include:

- Programming skills
  - Good programming practice
  - Languages: Fortran90, C++, Python
  - Builders and Visualisation
- Review of Classical Mechanics:
  - Lagrangians
  - Hamiltonians
  - Equations of motion
- Review of Quantum Mechanics:
  - Schrödinger's equation
  - One-dimensional wells and barriers
  - Central potentials: the hydrogen atom
- Review of Statistical Mechanics:
  - Thermodynamics
  - Probability distribution and partition function
  - Observables
- Electronic structure calculations
  - Basic many-body theory: Hartree-Fock and Density Functional Theory
  - Molecular orbitals and Bloch functions
  - Basis sets: plane waves and local orbitals
  - Pseudopotentials
- Force fields
  - Interatomic potentials and applications
  - Development, fitting and testing
- Simulation methods in Statistical Mechanics
  - Molecular dynamics
  - Monte Carlo
  - Calculation of Mechanical and thermodynamic properties

Learning outcomes
On completion of this module, the successful student will be able to

- Set up and critically discuss the theoretical framework to describe a material in a specified situation
- Write simple programs for simulation and analysis of results
- Perform electronic structure calculations and critically analyse the results from them
- Develop and critically test force fields for specific materials
- Run and critically analyse molecular dynamics and Monte Carlo simulations

Indicative time allocation

Structured study of course materials	40 hours
Electronic conferencing	40 hours
Assignments	80 hours
Independent learning time	40 hours

Assessment

Assignments	85%	On-line participation	15%

Supplementary notes

The module will be offered in a given year if a minimum of four students enrol on the module.

PHYxx30 Materials Science Research Project

Level and credits

Level M; 60 CATS.

Pre-requisites / Co-requisites

Fundamentals of Materials Science, Materials Characterisation and Materials Case Study

Module content

The project will take the form of an extensive research investigation into a topic relevant to materials science and engineering. This may involve evaluating a materials fabrication technique, analysing materials failure using a range of characterisation techniques or a systematic study of specific materials properties through experimental or simulation techniques. The results from the investigation will be analysed with appropriate conclusions drawn and presented.

Learning outcomes

On completion of this module, the successful student will have achieved the following learning outcomes, commensurate with module classification

- Deep knowledge and understanding of a specific research problem in materials science and engineering.
- Critically evaluate a research problem.
- Conduct a detailed analysis of the literature.
- Act autonomously and creatively in planning and implementing tasks.
- Critically analyse results.
- Communicate conclusions clearly.

Course components

Independent research project	600 hours

Assessment

Dissertation (50%), Continual Assessment (35%), Oral Presentation (15%).

Supplementary notes