DEPARTMENT OF MATERIALS

PART II PROJECTS

2022/2023

UNDERGRADUATE PART II PROJECTS

The project descriptions can also be found at:
www.materials.ox.ac.uk/teaching/part2/pt2newprojects.html

Further projects may be publicised at a later date.

There will be an open afternoon on Friday 25th February 2022 with introductory talks on Part II from the Part II Co-ordinator. Attendance at these talks is mandatory for all MS students commencing Part II in Michaelmas Term 2022.

Arrangements regarding supervisor availability on the day will be circulated beforehand.

Prospective Supervisors:

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PROJECTS ON OFFER:

1. Liquid lithium corrosion of materials for nuclear fusion

David Armstrong Co-Supervisor(s): Chris Grovenor

For nuclear fusion to be a commercial reality reactors must be self-sufficient in tritium. The only viable route for tritium production is through the capture of a neutron by a lithium atom which decays to helium and tritium. Liquid breeders use flowing liquid lithium alloys which has the advantage that tritium can be easily extracted, but the major disadvantage of the corrosive nature of liquid lithium.

This project will perform corrosion of alloys of interest to the fusion community, some provided by collaborators in the UK Atomic Energy Authority designing the STEP fusion reactor, and TaC coatings on steels prepared by sputtering. Samples will be examined using optical microscopy, SEM, EBSD and EDX. The aim will be to find alloys with good corrosion resistance, understand what corrosion products are produced and investigate the effect of different microstructures on corrosion resistance. This understanding will then be fed back to inform the engineers designing STEP.

2. Nanoindentation mapping of tungsten based intermetallics

David Armstrong Co-Supervisor(s): Angus Wilkinson, Junliang Liu

Tungsten is the leading candidate material for use for plasma facing components in nuclear fusion reactors. One projected use is as a sacrificial coating on steel substrates. However the iron-tungsten phase diagram contains multiple intermetallic phases of complex crystallography and unknown mechanical properties. Modern nanoindentation methods allow for mapping on the sub micron length scale.

In this project we will combine nanoindentation with SEM-EDX and EBSD to study formation of intermetallics in W-steel diffusion couples and their effects on mechanical properties. The project will be mostly experimental but with the potential for some matlab or python code development.

3. A model for radiation-curing of polymers

Hazel Assender

We have used various forms of radiation curing (UV, electron-beam, plasma) to polymerize diacrylate monomers to a solid, crosslinked polymer layer for coatings in functional materials and devices. Experimental data suggest that the degree of cure depends on the amount of radiation, but also the time it is applied and the depth of material. This project will seek to model these data and understand the crosslinking behaviour, and subsequent swelling and mechanical properties of the material. There is scope for practical work to generate more data as required, but the focus of the project will be on the creation of a model to link density of formation of reactive centres (radicals) with the nature of the cross-linked network.

4. Microchannel Electrodes for Implantable Neuronal Interfaces

Hazel Assender

This project, in collaboration with James FitzGerald, Dept. Surgical Sciences, seeks to develop a structured microchannel polymer that can be used as an interface to receive an array of neuron signals e.g. for prosthetics. The work will involve casting a structured PDMS material and vacuum-depositing metal electrodes in the microchannel structure and electrical testing, in vitro, and possible in vivo (rat) of the resulting devices. The incorporation of controlled-release drugs (e.g. anti-scarring) into the structure will also be considered.

5. Atom Probe Tomography investigations of liquid metal coolant uptake into nuclear fusion reactor components

Paul Bagot Co-Supervisor(s): Michael Moody, Christina Hofer, Andrew London (UKAEA)

Liquid metals are proposed as a coolant for the tritium breeding blanket component of future fusion reactors. Ceramic coatings prevent corrosion of internal metal components, and limit tritium uptake of these materials. Coated samples have been exposed to a lithium-lead liquid mixture. Diffusion of lithium through the coating is of key concern.

This project aims to characterise lithium in exposed coatings using atom probe tomography. APT can locate trace elements with high sensitivity and nm spatial accuracy, offering a unique potential to elucidate critical diffusion pathways and leading to improvements in coating technology. This project includes the exciting opportunity to collaborate with UKAEA's Materials Research Facility.

6. Visible photonic circuits for all-optical low-loss photonic computing

Harish Bhaskaran

7. Pockels effect in PCMs for integrated photonics

Harish Bhaskaran

8. Atomically thin planar metasurfaces based on nanostructured van der Waals materials

Harish Bhaskaran

Project descriptions to follow

9. Optimal Software Interfacing for quantum systems

Lapo Bogani

Quantum systems rely on a specific features to achieve performance, and the data treatment poses specific challenges and issues. In this project you will mostly interface with datasets that have already been acquired in order to decipher several of the quantum features of the materials. The project will see the development of dedicated software and will allow learning a variety of languages and tools oftentimes used in large data processing, such as mathematica, matlab, java, python etc... In this project you will push the current limits in how data are modelled and you will need to develop a solid scientific understanding of the underlying phenomena.

This is a project designed for a student who wants to improve their informatics and data treatment skills. You will learn how to model large datasets and the challenges associated, and you will need to understand the experimental challenges and the phenomena that are associated with the quantum systems. You will test what characteristics allow for optimal performance, and eventually you will learn the basics for large datasets representation and discussion.

10. Single-molecule Spin Spectroscopy

Lapo Bogani

One of the fundamental challenges of contemporary science is to be able to probe the behaviour of single atoms or molecules: investigating a single quantum system allows probing the interaction with the environment on the quantum behaviour, and testing our understanding of fundamental phenomena. The spin energy levels of a molecule are usually investigated by shining microwaves, so that the changes in reflectivity of a resonator is measured while a magnetic field is applied.

This project will test a completely different approach, in order to reach single-molecule sensitivity: the molecular states will be probed by single-electron-transport, while sending microwaves through the electrodes. In doing so, you will combine the techniques of single-molecule transport and electron paramagnetic resonance. You will have the possibility of learning nanofabrication, nanoelectronics, microwave optics, and cryogenics. You will test what device geometries allow for optimal performance, and eventually you will use the setup developed to measure samples of molecular magnetic materials.

11. The quantum properties of molecular graphenoids

Lapo Bogani

Graphene is a material with amazing structural, conducting and mechanical properties. On the other hand, it is still difficult to add one property to it: a magnetic behaviour. This is because graphene is, by itself, diamagnetic. We could recently introduce spin states into synthetic graphene nanostructures by chemical functionalization (Nature 2018) and topological manipulation (Science 2019). On the other hand, one ingredient remains missing: a sizeable spin-orbit coupling, which would allow mixing electronic and spin states so as to create truly multifunctional topological materials.

In this project you will investigate our next generation of graphene materials, where metal centres with high spin-obit coupling have been introduced. You will measure the quantum and classical spin properties using advanced pulsed electron paramagnetic resonance techniques, and interpret the results. In this project you will learn the basics of quantum information, advanced pulse techniques for their implementation, and the relevant data treatment. This is a project aimed at a student interested in learning advanced instrumentation, where most of the time will be spent on data acquisition and treatment.

12. Advanced Metallisation Technology for Next-Generation Photovoltaics

Sebastian Bonilla Co-Supervisor(s): Matthew Wright

Solar photovoltaic cells use metal contacts made primarily of screen-printed silver, and in some cell designs the metallisation also requires a transparent conducting film of indium tin oxide. The use of these materials is currently limiting further reductions in cell manufacturing cost, with the metals used contributing as much as one quarter of the cost of the cell. The ongoing trend to reduce the price of solar panels requires the shift towards a metallisation schemes that minimise the use of such expensive or nonabundant materials.

This project aims to explore novel contact and metallisation technologies that can address this critical hurdle for the future of solar electricity generation. Silver-free metal to semiconductor contacts will be explored in collaboration with our international partners, and new technologies will be proposed to achieve low-cost manufacturing of efficient metallisation for single and multijunction solar cells. This project requires hands-on electrical and optical measurements of materials, as well as data processing and analysis. Analytical and electrical characterisation techniques will be used to assess the performance of the metallisation, including advanced nano scale mass-spectroscopy and electrical current transport. The understanding and development from this project will result in improved manufacturing of commercial solar panels, which in turn will help mitigate the devastating consequences of climate change.

13. Studying the stability of charged oxide inversion layer (COIL) solar cells

Sebastian Bonilla Co-Supervisor(s): Matthew Wright

Over the past ten years, the cost of silicon solar panels has rapidly reduced, solar PV is now the best approach to displace fossil fuel electricity generation and cut CO2 emissions. The formation of a p-n junction in the silicon is critical for the operation of a solar cell. In industrial solar cells, the p-n junction is formed using an expensive, high temperature (> 700 °C) process in a furnace. An alternative approach, which is being developed in our group, is to deposit a layer of fixed charge in a dielectric layer, such as silicon dioxide. This could significantly reduce the temperature required to make the solar cell, however, for the technology to compete with existing designs, the introduced fixed charge must remain stable over the 25 year lifespan of the solar panel.

The aim of this project is to investigate the stability of the surface passivation and electron transport in charged oxide inversion layer (COIL) silicon solar cells. In particular, we require a better understanding of how the fixed charge will behave in the presence of elevated temperature and illumination with infra-red light. This project will generate a better understanding of how this new solar technology may perform under real-world operating conditions. This project will require hands-on measurements of the silicon materials in the laboratory as well as analysis of the generated photoconductance and photoluminescence data.

14. Field Effect Devices Based on Ion-Charged Dielectric Nanolayers

Sebastian Bonilla Co-Supervisor(s): Matthew Wright

Ion charged dielectrics are a class of thin-film material that possess a permanent charge. The charge storage capability of these materials makes them essential to a wide range of applications, from telecommunications to air filters and biomedical devices. At Oxford Materials, we have developed new methods to produce substantial concentrations of charge in dielectric thin films, in to fully exploit their potential in making of devices. This project aims to discover new dielectric-ion combinations and apply them to the manufacture of optoelectronic devices, like solar cells, photodetectors, and photodiodes.

The project will involve establishing a reproducible and controllable method of growing nanometre scale thin films using different synthesis methods, followed by delivery of new precursor ions, and their drive in into the dielectric. After the methodology is stablished the novel ion-charged dielectric systems can be integrated into devices, and their performance will need to be characterised. This project requires hands-on electrical and optical measurements of materials, as well as data processing, analysis, and modelling of the observed current transport characteristics. Ultrathin dielectric films will be employed in the next generation of silicon solar cells to produce architectures with minimum losses. As such this project feed in the Lab's aim of improving future photovoltaics technology to help accelerate the green energy transition.

15. DFT modelling of O-redox cathode materials

Peter Bruce

Lithium-ion batteries have revolutionised portable electronics and the demand continues to grow as transport is electrified. The cathode represents one of the greatest barriers to increasing the energy density of Li-ion batteries. In current cathode materials Li removal during charge is compensated by transition metal oxidation, limiting energy density. A new class of high voltage materials stores charge on both the transition metals and oxide anions, potentially offering a 50% increase in energy density. However several problems prevent their application, including structural changes, oxygen loss, slow kinetics and capacity fade. This project will use DFT to investigate the changes taking place in these cathode materials. This will help to provide valuable insight into the processes underpinning anionic redox.

16. Polymerisation of casein

Jan Czernuszka

Casein is a naturally occurring protein. This project will examine ways to form solid structures. The resultant mechanical properties will be measured and related to methods of production.

Refs: Current opinion in Colloid and Interface Science Vol 7, (2002) 456.

17. Optimising the prepreg production for an Alumina based Oxide Ceramic matrix composite

Marina Galano Co-Supervisor(s): James Marrow

The proposed Part II project aims to use the findings and characterisation techniques developed in a previous project to further optimise the microstructure and creep resistance of oxide-oxide ceramic composites, CMCs, by nano-engineering of the matrix for improved creep resistance at elevated temperatures. The project would involve modifying an already existing matrix slurry system in order to enhance the creep properties of the CMC system. Samples would be produced which would then be passed through a test matrix in order to fully quantify their mechanical properties.

The objectives of this project are i) manufacture oxide-oxide ceramic composites on a pilot scale at Oxford, and ii) achieve and verify a further improvement in creep resistance through nano-engineering of the microstructure.

18. Effect of the Strain rate on high cycle fatigue of titanium alloys

Jicheng Gong Co-Supervisor(s): Angus Wilkinson

Fatigue is the most pervasive failure mode across the industrial sectors. Our group developed a novel fatigue testing technique that can assess a small volume of material at an extremely fast rate of 20 KHz, enabling a high cycle fatigue (HCF) test in hours in contrast to months using the conventional approach.

This project will investigate the influence of the testing rate (strain rate) on HCF crack initiation and short crack growth in titanium alloys by comparing the ultra-small & ultra-fast fatigue test with a low frequency meso-cantilever test. Two SN curves will be achieved. Intermittent and post-mortem analysis by SEM and EBSD characterisation will be conducted to underpin the fatigue behaviour and properties as a function of the strain rate. Static meso-cantilevers can be deflected by the nanoindenter to measure the load-displacement response. Strain rate jump tests and DIC analysis will be performed in these static meso-cantilevers to establish the correlations between the strain rate and plastic deformation with respect to the microstructure. The results will be used to interpret the effect of strain rate on HCF and dwelling fatigue in titanium materials. Finite element model will be implemented to simulate the dynamic response of a cantilever and calculate the stress in an ultrasonic fatigue test.

19. Li alloys for solid state batteries

Chris Grovenor Co-Supervisor(s): David Armstrong

Storing the highest energy densities in solid state Li batteries requires the use of metallic Li as the anode, but Li metal is very soft, extraordinarily reactive and difficult to use in practical devices. One idea to improve the properties is the formation of high Li content alloys. The simple Li-Mg binary system has a wide solid solution range, and has been studied extensively, but does not offer the solution to all the practical difficulties.

This project will make and test novel ternary alloys (with Al, Mg, Sn, Si, Zn) designed to allow the microstructure/mechanical properties and electrochemical performance to be controlled independently. Samples will be examined using optical and SEM, EDX and XRD techniques to establish the as-cast microstructure, to measure the mechanical properties, and the more promising materials will be selected for electrochemical testing. If the student is interested, they could learn how to use Thermocalc software to predict ternary phase diagrams for the selected alloys, and to compare these predictions with the real phase mixtures.

20. Synthesising New High Energy Cathodes for Mg-ion Batteries

Robert House Co-Supervisor(s): Peter Bruce, Saiful Islam

Magnesium ion batteries are a promising, sustainable alternative to conventional Li-ion. Besides offering lower cost, Mg-ion could also potentially offer higher energy densities than Li-ion. Since Mg^{2+} is a divalent carrier-ion, each ion can transfer twice the charge (or more) as Li^{+} ions, doubling the charge storage per ion. However, there remains only a limited number of known cathode materials for these batteries.

New sulphide cathode materials will be synthesised and tested in Mg-ion battery cells. XRD, SEM and a range of electrochemical characterisation tools will be employed to understand their charge storage behaviour. There will also be an opportunity for the student to explore computational methods to support their experimental results.

21. Stabilising O-redox in Disordered Rocksalt Battery Cathodes

Robert House Co-Supervisor(s): Peter Bruce, Saiful Islam

Disordered rocksalts are a new class of high-performance cathode material for rechargeable batteries. Based on the cubic NaCl structure, materials such as Li_2MnO_2F can be made with a disordered arrangement of Li/Mn on the cation and O/F on the anion sites in the lattice. These materials exhibit high energy densities supported by oxidation and reduction of oxide ions (O-redox), but also gradual degradation over cycling associated with this reaction.

The student will explore the effect of various elemental substitutions into Li_2MnO_2F to stabilise the O-redox reaction. Ball-milling synthesis and various characterisation tools including XRD, SEM and X-ray spectroscopies will be employed. There will also be an opportunity for the student to link up with computational work in this area.

22. Dynamic mechanical analysis of 3D printed reinforced polymers

Colin Johnston Co-Supervisor(s):Enzo Liotti & Vitor Marques (Leonardo, UK)

3D printed parts are now moving into production however there remains some concerns about the strength and durability of 3D printed parts, especially for the aerospace sector. This project aims to use dynamic mechanical analysis (DMA) to look at how fibre reinforcement improves the stiffness and strength of 3D printed polymer parts, in particular comparing the performance of printed Onxy (chopped fibre reinforced nylon) and continuous fibre reinforced Onxy against non-reinforced nylon. The stress/strain properties will be measured as a function of temperature and frequency. The microstructure and distribution of the reinforcement will also be investigated.

The project is support by Leonardo UK a global aerospace company who will supply 3D printed parts. However, there is also an opportunity to use our own 3D printers to produce parts for testing.

23. Scalable HRTEM image simulation of nanoparticles for machine learning dataset generation

Angus Kirkland Co-Supervisor(s): Chen Huang

Machine learning has become an important technique in image analysis of large datasets. However, few existing experimental electron microscope image datasets are suitable for the training of deep neural networks due to the high cost of data labelling. However, with careful configuration, high resolution transmission electron microscopy (HRTEM) simulation is now able to closely match the experimental HRTEM images and is therefore ideal for creating the huge training datasets required.

The goal of this project is to streamline the model generation and image simulation process for nanoparticles with ultimate goal of being able to use this in the analysis of catalyst materials. The initial aim is to reduce the current computation time by at least an order of magnitude, by carrying out simulations of a variety of particle morphologies, orientations and sizes using to the university's Advanced Research Computing (ARC) facility. This project would suit a student with an interest in computation and model building and will involve a moderate amount of programming. Basic familiarity with MATLAB is essential. Some knowledge of nanoparticles and TEM are ideal but are not essential.

24. Atomic resolution electric field mapping

Angus Kirkland Co-Supervisor(s): Christopher Allen

Due to the dimensional constrains of a nano-electronic device, any deviation from a perfect crystal lattice can have profound consequences on its electronic characteristics. These deviations can take the form of defects in the crystal lattice, substitutional/interstitial dopant atoms, or edge/surface structure. Modern transmission electron microscopes (TEM) have made imaging the atomic structure of a wide range of nano-materials fairly routine. From this experimentally determined atomic structure the theoretical internal electric fields can be calculated and electronic characteristics predicted. Recent advances in TEM detector technology now enable the direct imaging of internal electro-magnetic fields in nano-materials at atomic resolution.

To achieve this an electron probe is focused onto the sample surface in a standard scanning-TEM (STEM) experiment and the far-field diffraction pattern recorded at each electron probe position. Any deflection in the forward scattered bright field disk is related to a momentum transfer from the internal electro-magnetic field of the material to the electrons in the probe. By measuring changes in the intensity distribution of the bright field disk in the recorded diffraction patterns the internal electric field of the material can be calculated. In general these experiments are performed at a reasonable high electron dose in order to ensure good signal to noise ratio in the recorded diffraction patterns. However this high electron dose transfers significant energy to the sample and can cause bond breaking and atom ejection changing the very atomic structure being investigated.

In this project you will explore the low dose limit of atomic resolution electric field mapping. Firstly using established code you will simulate data-sets under a variety of low dose conditions and then reconstruct the internal electric field and compare with calculations in the literature. This will require significant coding (in Python and Matlab) and a strong mathematical background. You will then go on to look at experimental low dose data taken from MoS_2 across a range of incident electron doses to explore when the technique breaks down under real experimental conditions.

As a significant amount of experimental data has already been collected for this project we envisage that the bulk of this project will be simulation and data analysis including extensive coding. Depending on progress there may be the opportunity to collect more data either on the ARM200CF in the Materials Department at Parks Road or on the ARM300CF at the electron Physical Sciences Imaging Centre at Diamond Light Source.

25. Intrinsic flow constriction methods for gravity casting filling system design

Enzo Liotti

In gravity casting the design of the filling system is crucial to obtain high quality components. Ceramic filters are ubiquitously used in industry to reduce turbulence, however for large casting their effectiveness is often not satisfactory and turbulent flow can occur with all the detrimental consequences for the quality.

The project will explore, using 3D fluid-dynamics simulations, alternative flow constriction solutions, such as honeycombed channels and Tesla valves, to actively control the liquid velocity without the use of ceramic filters. The performance of the most promising solution will be tested on Aluminium alloys in a small-scale laboratory experiment.

26. High-resolution characterization of metal powders for Additive Manufacturing of space materials

Sergio Lozano-Perez Co-supervisor(s): Neil Young

This project is in collaboration with the European Space Agency (ESA), which has an interest on using additive manufacturing for producing space hardware. One topic of particular interest is the control of the raw material. Metallic powders can be produced in different grades of quality and only the highest performing powder is selected for producing space parts. This Part II project aims to improve the understanding of powder characteristics by utilising methods such as Focused Ion Beam (FIB), high resolution Electron Microscopy (SEM) and related analytical methods (EDX).

27. Synchrotron X-ray imaging and diffraction analysis of tensile deformation of a ceramic composite

James Marrow

3D needle-punched carbon fibre felts or non-woven cloths are used as the reinforcement in C/C and C/C-SiC composites. To understand how damage tolerance is affected by process variables (e.g. thermal stresses) and composite architecture, it is important to observe how damage initiates and propagates (doi.org/10.1016/J.COMPSTRUCT.2018.11.041). This project asks the question "How does damage in the matrix and fibre bundles interact with the process-induced residual stresses?". This information is needed to validate image-based models of composite behaviour (e.g. doi.org/10.1111/ffe.12537). A unique experiment at the Diamond Light Source examined the tensile deformation of a 3D needle-stitched C/C-SiC ceramic composite. In situ high resolution computed tomography was combined with high energy diffraction to examine cracking and stress partitioning in the composite constituents.

This is a data analysis project, so no new experiments will be done. You will need to develop an approach that combines 3D strain mapping by digital image correlation of tomographs with 2D mapping of the crystal strains by analysis of monochromatic Bragg diffraction data (e.g. doi.org/10.1016/j.carbon.2020.03.020) to correlate the evolution of stress, strain and damage in a large and complex dataset. You will use state-of-art visualisation (Avizo) and diffraction analysis (DAWN) tools, and have the opportunity to develop novel data visualisation and numerical analyses.

28. In situ Studies of the Deformation of Highly Porous 3D CNT tube (CNTT) Networks

James Marrow Co-Supervisor(s): Nicola Pugno (University of Trento)

Highly porous 3D CNT tube (CNTT) networks have interesting mechanical and electrical properties with potential applications in technologies that include stretchable conductors, gas sensing, cell-scaffold materials, and cathode materials for batteries. A novel material has been developed (at Keil University) with mechanical properties and electrical properties that are enhanced by CNT networks, self-entangled around a highly porous 3D zinc oxide ceramic 'tetrapod' foam (https://doi.org/10.1038/s41467-017-02372-9). It has an open structure with a high porosity, which is beneficial for several applications due to high surface accessibility. The ceramic can be dissolved to leave the CNTT network.

This project asks the question "How does the network deform, and is it uniform or heterogeneous?" This question can only be answered by in situ observations, obtained within the three-dimensional material. You will design experiments to study the cyclic deformation and failure of CNTT materials, using in situ, high resolution computed X-ray tomography. Deformation and fracture will be quantified using digital volume correlation, as a function of the applied strain. The project will involve mechanical testing, computed tomography, data visualisation and numerical analysis (Matlab), with opportunities to apply finite element simulation.

29. Indentation Damage in Advanced Ceramics and Composites

James Marrow

Indentation damage in ceramics is a complex process that includes elastic and inelastic deformation as well as brittle fracture (doi.org/10.1016/j.jeurceramsoc.2014.04.002). It forms the basis of several standard tests for measuring the mechanical properties of ceramics and is also highly relevant to practical applications such as light weight armour and the wear of high temperature cutting tools.

However, the details are still not well understood, which impedes the design of damage resistant ceramics and composites. This is partly because it is very difficult to study the processes that occur under the indention. One method for studying the internal structure of materials is X-ray computed tomography (XCT), which can be applied with sub-micron resolution to materials that are opaque to visible light; the obtained 3D datasets can be analysed by digital volume correlation methods (DVC) to measure the full field displacements that arise from damage and cracking.

This project asks the question “Can the characteristic fracture toughness of a ceramic composite be obtained via measurements of the 3D displacement fields of cracks at indentations?” To address this, you will design experiments to compare non-destructive. XCT/DVC analysis of indentation tests, observed in situ, with destructive post-test analysis methods that characterise the damage by optical and electron microscopy. Emphasis will be placed on the measurement of the modes of crack opening (i.e. tensile/shear) and the strain fields around cracks which may be used to obtain the criteria for crack propagation. The analysis will require some use of finite element modelling methods, and also post-processing of data using tools written in Matlab.

30. Atmospheric Pitting Corrosion and Stress Corrosion Cracking of Stainless Steel

James Marrow Co-Supervisor(s): Marina Galano

Salt contamination on the surfaces of stainless steel components can develop very high concentrations of chloride ions under certain combinations of humidity and temperature. This can create the conditions for pitting corrosion (dx.doi.org/10.1149/1.3407553).

The pits are stress concentrations, from which stress corrosion cracks may initiate if there is a sufficient mechanical load. Welded components, such as the stainless steel flasks that store intermediate nuclear waste, may contain significant residual stresses, and additional loads may develop if there is a changes in the dimensions of their contents; hence there is a potential risk of failure. Predicting the likelihood of failure needs data for the time to initiate pits and the criteria for crack initiation. This project asks the question “Does the criteria for crack initiation depend on whether the pit develops under stress, or if the stress is applied after the pit has developed?” This experimental study will examine the development of pits on salt-contaminated stainless steel under controlled conditions of humidity and temperature; selected pits will be characterised by high resolution computed tomography. The time to develop cracks will be examined in statically loaded specimens (U-bend) that have been pre-pitted before loading, or have no initial pits. In situ observations, analysed by digital image correlation, may also be performed to examine the kinetics of crack growth. This project does not necessarily require any numerical modelling.

31. Analysis of in situ high resolution synchrotron tomography of graphite fracture

James Marrow

Graphite is used as a neutron moderator in high temperature nuclear reactors. Its fracture toughness depends on the relative strengths of the filler particles and binder matrix, which may age differently. Multi-dimensional observation and analysis of crack propagation can be used to study fracture resistance (http://dx.doi.org/10.1016/j.carbon.2020.09.072). A recent tomography experiment at the PSICHE beamline of the SOLEIL light source (20190926) has obtained images for crack propagation in nuclear graphite at unprecedented spatial and temporal resolution and with large field of view. This project asks the question “Can the local fracture resistance of matrix and filler within the heterogeneous and porous graphite structure be quantified?” This is a data analysis project, so no new experiments will be done. You will need to devise an efficient analysis method to extract and correlate the crack’s 3D strain fields with their local microstructure using a large dataset. You will also apply state-of-art visualisation, machine-learning based segmentation and digital correlation analysis software (Avizo). The output will lead to improved modelling of the strength of nuclear graphites.

32. Atomic scale characterisation of non-equilibrium precipitate evolution in Applications

Michael Moody Co-Supervisor(s): Paul Bagot, Yuanbo Tang

Additive manufacturing (AM) is particularly relevant to the Ni-based superalloys. AM can produce fragile structures required for certain higher temperature and lightweight applications that were not previously possible with the conventional processing route. However, to improve applicability, a fundamental understanding must be established, at the atomic-scale, as to the nature of the microstructures that are promoted or inhibited by the extremely fast heating and cooling rates generated using this approach.

The project will apply state of the art atom probe tomography to investigate gamma prime evolution in terms of composition and volume fraction in novel alloys designed at Begbroke. To this end, a range of post-processing treatment conditions will be investigated to gain insight into the kinetics of phase transformation so as to fully exploit the process advantages offered by AM.

33. Controlling damage in electron microscopy characterization of polymers

Pete Nellist Co-Supervisor(s): Hazel Assender

Electron microscopy can provide structure characterisation up to atomic resolution, and is widely applied for inorganic materials. For organic materials, such as polymers, the limiting factor is the rapid damage that can occur to the sample under electron irradiation. Recent developments in scanning transmission electron microscope (STEM) imaging methods have shown the potential to provide high-resolution characterisation of polymers with reduced damage. Why the type of illumination in STEM reduces damage is not well understood, and this project seeks to build this understanding which would unlock new ways to characterise polymer structures and other molecular crystals. The project will involve preparing polymer test samples and then using electron microscope imaging and diffraction to characterise the damage that is occurring under different types of illumination.

34. Graphite anodes for K-ion batteries

Mauro Pasta Co-Supervisor(s): Krishnakanth Sada

Due to the rapid battery market expansion and the limited and geographically concentrated lithium and cobalt resources, there is significant concern regarding the short-term supply and long-term sustainability of lithium-ion batteries. Potassium-ion batteries (KIBs) are emerging as a promising complementary technology to LIBs due to the relative abundance of potassium [Dhir, Wheeler, Pasta et. al., *Chem* (2020)]. KIBs can also use graphite anodes providing a critical advantage over sodium-ion batteries.

The mechanism of K-ion (de)intercalation in graphite has been studied extensively in the literature [Hosaka, Komaba et. al.; *Chem Rev* (2020)]. However, the role of crystallographic defects is still mostly unexplored [Igarashi, Komaba et. al. *Electrochemistry* (2021)].

In this project, the student will employ *ex-situ* and *in-situ* Raman spectroscopy and X-ray powder diffraction and electrochemical characterisation techniques to investigate the effect of crystallographic defects in graphite on intercalation mechanism, K-ion transport and long-term cycling.

35. Solvation structure of fluoride-ion electrolytes

Mauro Pasta Co-Supervisor(s): Hua Guo

The climate crisis is driving the search for novel battery chemistries that can power high-energy applications, such as electric vehicles and electric flight. Among the available candidates, fluoride-ion batteries (FIBs) are a promising technology because of their high theoretical energy density and utilization of abundant and widespread materials. However, FIBs present several new challenges that are preventing them from reaching commercialization [Xiao, Galatolo, Pasta *Joule* (2021)]. The lack of a suitable electrolyte is arguably one of the toughest to address. Although a few promising liquid electrolyte systems have recently been reported [Davis, Jones et. al. *Science* (2018), Koishi, Ogumi et. al. *Chemistry Letters* (2018)], there is still a lack of understating of the link between solvation structure, ion transport and degradation mechanism.

In this project, the student will investigate the solvation structure of F-ion in different solvents and solvent mixtures by Nuclear Magnetic Resonance (NMR) and Raman spectroscopy. The effect on solvation and F-ion transport will be explored by Pulse-Field-Gradient (PFG) NMR.

36. Characterisation of Li-ion battery materials

Mauro Pasta Co-Supervisor(s): various materials engineers at Northvolt

The project(s), carried out at Northvolt's laboratories in Sweden and under the direct supervision of a battery materials engineer, aim at exploring the physicochemical and electrochemical properties of novel battery materials, including:

- Binders;
- Silicon-based anodes;
- Electrolytes;
- High-capacity cathodes;

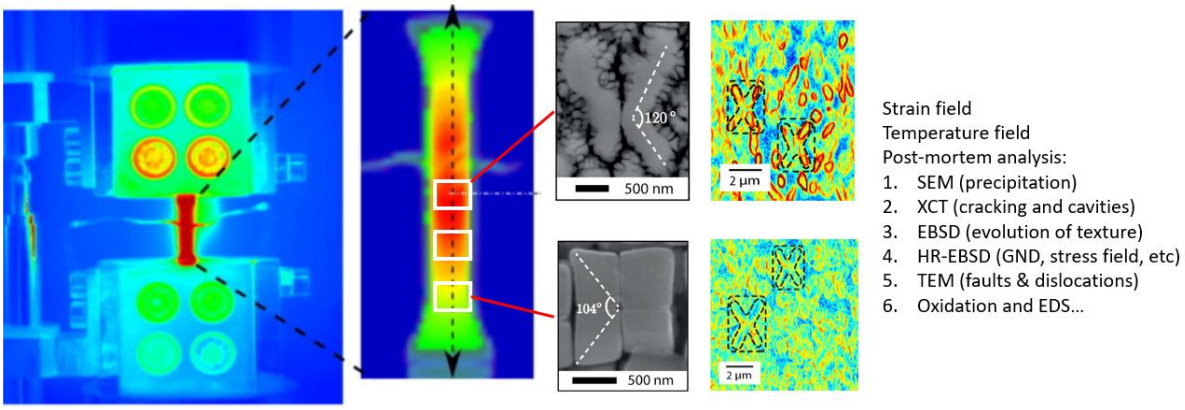
The student(s) will apply fundamental materials synthesis and characterization concepts learned in their PartI and develop new skills in electrode fabrication, cell assembly and electrochemical testing.

37. On the high throughput multi-field characterisation of deformation in Ni-based superalloys

Roger Reed Co-supervisor (s) : Yuanbo Tang

Creep, inelastic time-dependent deformation, is one of the limiting properties for high temperature applications. However, the standard creep measurements require a large amount of material and are notoriously long-winded and costly. This is particularly undesirable when materials availability is unabundant, such as for the development of new alloy compositions. High throughput testing takes the advantage of miniaturised designs has been under development for reliable rapid assessment. In this project, we build upon the previous success of utilising an electro-thermo mechanical testing system to characterise the deformation behaviour of fine grain and single crystal superalloys.

In contrast to a conventional isothermal environment, we assess creep property in a sample presented to a temperature gradient with uniaxial loading. An innovative multi-field correlative set-up is designed to couple thermal field and strain field measurements as a function of accumulative plasticity. The microstructural evolution will be characterised using high resolution microscopy, with an emphasis on the evolution of cavitation, texture, precipitation and local lattice rotation. The ultimate goal of the project is to acquire a large dataset to establish constitutive laws and to construct a deformation map using only few samples.



38. Characterisation of ultrafine aerosol particles using single photon detection

Jason Smith

Atmospheric aerosols of size below 1 um, known as ultrafine particles or UFPs, are increasingly recognised as major causes of illness and mortality in urban areas, but they are difficult to detect using traditional light scattering methods as the scattering efficiency is extremely low. This project will use a newly developed detection system for UFPs and assess its ability to characterise the particles in terms of their size and composition.

39. Compact nutrient sensors for water quality monitoring.

Jason Smith

Nutrients such as nitrates and phosphates are major sources of pollution in waterways, causing algal blooms and threats to health, and there is a global need for improved sensors to monitor their levels. In this project you will build and test a new design of a compact optical sensor based on microcavity technology developed within the group. The project will be carried out in communication with spinout Oxford HighQ Ltd with a view to its potential for industrial application.

40. Magnetic biasing of solid state spin qubits

Jason Smith

Spin qubits such as the NV centre in diamond require biasing with a fixed magnetic field which must be aligned accurately with the axis of symmetry of the crystal defect. This project involved the design, building and testing of a device that will provide biasing for NV centre qubits in experiments at ambient and cryogenic temperatures. The project will take place within a team working in the UK Hub for Quantum Computing and Simulation.

41. Persistent joints in high temperature superconductors

Susie Speller Co-Supervisor(s): Chris Grovenor, Tayebeh Mousavi

The large magnets required for applications in medical MRI and large physics experiments like the LHC at CERN are all based on superconductors, and can contain numerous joints that are often the (very expensive) points of failure. Reliable processing strategies are needed to prepare joints between shorter lengths of wire with resistances lower than 10^{-13} W.

This project will work with our partners in Oxford Instruments on making and testing joints between Bi-2212 superconducting wires – how to improve reliability and performance, and understanding what goes wrong. The project will involve improving joint making processes that are based on a melting and peritectic reaction process, using XRD and analytical SEM to analyse the phase purity and microstructure of the joints, and measuring the persistent performance of small coils by measuring the decay of induced currents.

42. Radiation damage in high temperature superconductors

Susie Speller Co-Supervisor(s): Chris Grovenor

High temperature superconductors (HTS) are an enabling technology for the next generation of compact nuclear fusion reactors that require very high magnetic fields to confine the plasma. In service, the superconducting magnets will be exposed to a flux of high energy neutrons, and little is known about how their performance will degrade under operating conditions.

This project will study how irradiation affects the structure and properties of HTS thin films, using ions as a safe proxy for neutrons. The student will fabricate thin film samples using pulsed laser deposition and will investigate structural changes using X-ray diffraction as well as assessing the effect on superconducting properties. There will also be opportunities to be involved in X-ray absorption experiments at Diamond Light Source.

43. Gradient flash sintering of ceramics

Richard Todd

Flash sintering is a novel method of ceramic processing involving heating and simultaneous passage of a current through the sample. The thermal gradients involved are usually seen as a problem to be minimised but if optimised could enable the production of novel microstructures and properties. Project will involve ceramic processing, microstructural investigation and mechanical testing.

44. Nacre-like alumina by interfacial optimisation

Richard Todd Co-Supervisor(s): Guillaume Matthews

The availability of cost-effective single crystallise alumina platelets has enabled the facile production of nacre-like microstructures with improved damage tolerance. However, the weak interfaces between the platelets still need to be optimised. The aim of the project is to try various treatments/additives to improve the toughness of these materials. Project will involve ceramic processing, microstructural investigation and mechanical testing.

45. Advanced Metallisation Technology for Next-Generation Photovoltaics

Andrew Watt Co-supervisor(s): Sebastian Bonilla

Solar photovoltaic cells use metal contacts made primarily of screen-printed silver, and in some cell designs the metallisation also requires a transparent conducting film of indium tin oxide. The use of these materials is currently limiting further reductions in cell manufacturing cost, with the metals used contributing as much as one quarter of the cost of the cell. The ongoing trend to reduce the price of solar panels requires the shift towards a metallisation schemes that minimise the use of such expensive or nonabundant materials.

This project aims to explore novel contact and metallisation technologies that can address this critical hurdle for the future of solar electricity generation, using solvo-dynamic printed nanowire high aspect ratio contact electrodes. Silver-free metal to semiconductor contacts will be explored in collaboration with our international partners, and new technologies will be proposed to achieve low-cost manufacturing of efficient metallisation for single and multijunction solar cells.
Analytical and electrical characterisation techniques will be used to assess the performance of the metallisation, including advanced nano scale mass-spectroscopy and electrical current transport. The understanding and development from this project will result in improved manufacturing of commercial solar panels, which in turn will help mitigate the devastating consequences of climate change.

46. Quantum Dot Photovoltaics

Andrew Watt Co-Supervisor(s): Sebastian Bonilla

The efficiency of solution processed lead chalcogenide colloidal quantum dot (CQD) solar cells has increased from less than 1 to over 15% in the last 12 years. They have proven to be air-stable and do not require high temperature processing, which are major drawbacks for competing thin film, organic, perovskite and dye sensitized technologies. A project is offered with one of the following focuses 1. CQD Syntheisis 2. CQD Device Characterisation 3.CQD TEM. All projects will involve the fabrication of devices.

47. Metal Nanowire Based Devices for Ambulatory Blood Pressure Monitoring

Andrew Watt Co-supervisor(s): Prof Helen Townley (Women's Reproductive Health)

Recently we demonstrated that we could build a nanowire-based pressure sensor with sufficient sensitivity and mechanical properties to measure changes in venal flow. We wish to build upon this exciting initial result and show that it is possible to make a passive measurement of blood pressure. The project will involve nanowire synthesis and device fabrication alongside ex vivo testing and a variety of materials characterisation techniques.

48. Direct-formation of suspended 2D material membranes

Robert Weatherup

X-ray Photoelectron Spectroscopy is one of the most powerful techniques for obtaining surface-sensitive chemical information, by detecting photoelectrons that escape from within a few nm of a surface. However it is typically restricted to solid surfaces under vacuum conditions, limiting its potential applications.

This project will involve the development of ultra-thin and impermeable 2D material membranes (Graphene/Tungsten Disulphide) for encapsulating liquids, so that they can be measured using XPS. This will include learning to produce 2D materials by chemical vapour deposition (CVD), and then optimising growth on metal layers suspend on perforated supports. The metal can then be etched away to leave the suspended 2D material membrane. These will then be characterised optically and with scanning electron microscopy before testing in a vacuum chamber to confirm they are leak-tight. They can then be used for observing liquid-phase catalytic reactions or the accumulation of ions on the surface of the 2D material under electrochemical bias using lab-based XPS systems in the department.

49. Revealing edge sites in graphite electrodes for Li-ion batteries

Robert Weatherup

Graphite is widely used as the anode in lithium-ion batteries, where lithium can be repeatedly inserted and removed from between its layers as the battery is charged and discharged. Alongside this reversible reaction, irreversible electrolyte decomposition can occur at the graphite surface. The extent of these irreversible reactions are thought to be significantly increased by the presence of graphite edges. Understanding the performance of different graphite electrodes thus requires an understanding on the proportion their surface associated with graphite edges compared to the less reactive basal plane.

This project aims to develop a straightforward approach to determine this based on the enhanced catalytic activity of these edges. Electrochemical reactions will be used to study well-defined graphene layers to determine the relationship between reaction rate and edge density. This will then be extended to a variety of commercially available graphite electrodes.

This will involve correlating electrochemical data with experimental characterisation of microstructure (Electron and optical microscopies) and surface area (BET method). Ultimately the aim is to correlate edge density with the irreversible capacity lost in real Li-ion batteries.

50. Size-selected alloy nanoparticles for electrochemical hydrogen production

Robert Weatherup

The production of hydrogen by electrochemical splitting of water offers a zero-carbon method for converting renewable energy to a fuel which can be stored for when it is needed and used to replace fossil fuels in many industrial processes. To produce hydrogen efficiently, electrocatalysts are needed that reduce the overpotential and avoid large amounts of energy being wasted. Alloy nanoparticle catalysts are particularly promising as they offer high surface areas, and their catalytic performance can be tuned by their size and composition. However, rational improvement of performance requires the deposition of a large number of nanoparticles of well-defined size and composition.

This project will use a newly acquired deposition source, that forms nanoparticles of controlled size by expanding a metal vapour through a nozzle, and then mass filters these to select only particles of a desired size. The formation of binary alloy particles will be studied and then their sizes and variation in composition characterised using electron microscopy, and X-ray photoelectron spectroscopy. The performance of optimised catalysts will then be investigated for electrochemical water splitting.

51. Effects of hydrogen on mechanical behaviour of steels

Angus Wilkinson Co-Supervisor(s) David Armstrong, Phani Karamched

Zero carbon energy systems are needed urgently. Gas is used for heating in 85% of households in the UK and this could be replaced by hydrogen supplied through the existing national transmission system (NTS). Assessing the potential effects of hydrogen on pipeline steels is a necessary part of the safety case. Ferritic-pearlitic steels are used in the main high-pressure pipelines and potential detrimental effects include hydrogen embrittlement and accelerated fatigue crack growth.

This project will compare the mechanical behaviour of such steels with and without hydrogen charging. Combinations of ex-situ and in-situ mechanical testing, with digital image correlation (optical and SEM imaging), will be used along with HR-EBSD, EDX and possibly AFM characterisation.

52. 3D Printing on the Moon - Micromechanical Evaluation of Lunar Regolith for Moon based Additive Manufacturing

Angus Wilkinson Co-Supervisor(s): David Armstrong, Christopher Magazzeni (ESA)

As human spaceflight returns its focus to the moon, creating safe longer-term habitats will be necessary. In situ resource utilisation (ISRU) would seem a requirement and one possible route is to create 3D printed structures from local lunar regolith material (soil). Advances have been made in mimicking in-space processing so that simulated 3D printed materials and structures are available.

The project consists of characterising simulated lunar regolith with the aim to understand its properties for such as additively manufacturing a moon base. Correlative nanoindentation and surface microscopy methods will be used to explore chemistry-structure-properties relationships at the microscale with the aim of developing better micromechanical understanding of these unusual materials. The project will involve close collaboration with engineers at the European Space Agency.

53. Crystal plasticity modelling of creep in lithium

Angus Wilkinson

Lithium metal anodes are being explored for both liquid- and solid- state electrolyte battery technologies. Mechanical properties of Li, particularly the creep response, is of technological importance in understanding and potentially mitigating the formation of voids during stripping and/or so-called dendrites during plating both of which degrade performance. The large elastic anisotropy of Li may drive considerable grain to grain variations in stress, strain and thus creep response at the microstructural level which seems to have been entirely unexplored to date.

The intensity, spatial size, and frequency of local ‘hot spots’ in stress, and strain in a simulated Li polycrystal under creep conditions will be explored using crystal plasticity simulations. Simulations will be benchmarked to data in the literature and on-going experimental campaigns in Oxford.

54. Computational Polarised Light Microscopy: Rapid micro-texture mapping

Angus Wilkinson

For non-cubic systems microscopy with polarised light offers the potential for rapid and easily accessible mapping of crystallographic alignment. Best acquisition and analysis routes combining images obtained with different linear and circular polarisation states will be explored in terms of speed, reliability and accuracy. Student input to materials to be analysed is welcomed (metallurgical, bio, geological…). However, an area of significant interest is in determining the size, shape, and alignment of ‘macro-zones’ or ‘micro-textured regions’ (MTRs) in Ti alloys. These MTRs are extended regions of similarly oriented alpha grains inherited from larger beta grain structures during processing and have been implicated as detrimental features in cold dwell fatigue failures.

55. Structural studies of supported metal nanoparticles and catalyst materials

Neil Young

The atomic structure of metal nanoparticles is of direct importance to numerous nanotechnology applications. Combining direct visualisation of nanoparticle structure via high-resolution TEM, with in-situ and ex-situ heating allows for nano-structural phase diagrams to be established. These give a thermodynamically robust account of nanoparticle atomic structure as a function of size and temperature. You will continue the work of previous PtII students on gold and silver nanoparticles, and extend this to include the influence of a range of support materials. You will study a range of commercial catalyst materials and formulate nano-structural phase diagrams for these systems.

56. Understanding ion damage in TEM specimen preparation, comparing Ar, Ga and Xe ions.

Neil Young Co-Supervisor(s): Ian Griffiths, Gareth Hughes

Artefact-free specimen preparation is essential in performing advanced materials characterising via electron microscopy. In this project you will use a recently installed Ar-ion milling system to explore the interaction of Ar ions with a range of TEM-ready specimen geometries.

The role of Ar-ions in polishing semiconductor specimens and removing artefacts will be explored via a systematic approach. As the project progresses FIB techniques will be introduced allowing the damage rate from Ar, Ga and Xe ion beams to be compared. The project would suit a student with a deep interest in materials characterisation techniques and instrumentation. An organised and careful approach to practical work would be required. The student would gain hands-on skills across a range of electron microscopy techniques and practical specimen preparation.

57. The application of density functional theory for the interpretation and optimisation of electron microscope imaging of chemical bonding

Pete Nellist Co-Supervisor (s): Jonathan Yates, Rebecca Nicholls

Recently developed imaging methods in electron microscopy have reached the level of precision where charge variations due to bonding can be detected. This image data can be quantitatively interpreted by comparison with density functional theory calculations. It has been shown that this approach is feasible in perfect crystals. The current question is whether charge redistribution at defects, as a result of dangling bonds for example, can be detected. The aims of this project are to model both the charge redistribution and the imaging process to determine the materials types and defects types that can feasibly be detected.

58. DFT modelling of transmutation products in neutron irradiated SiC

Rebecca Nicholls Co-Supervisor(s): David Armstrong

Silicon carbide composites (SiC) are under active consideration for a range of applications in future nuclear fusion reactors. In these environments they will subjected to damage from 14 MeV neutrons which will cause significant levels of transmutation and very little is known about the effects impurities produced in this way will have on SiC. Electron Energy Loss Spectroscopy (EELS) is the most promising method of studying the subsequent chemical segregation in the material, but the expected spectra are unknown. In this project, density functional theory will be used to understand the stable defect configurations in SiC and the effect this will have on EELS data.

59. DFT modelling of rare earth superconductors

Rebecca Nicholls Co-Supervisor(s): Susie Speller

Rare earth superconductors are the material of choice for generating very high magnetic fields in the next generation of nuclear fission reactors. The superconductor will be exposed to high energy neutrons so it is important to understand the defect structures that result. X-ray absorption spectroscopy is a very sensitive probe of chemical environment, but can be difficult to interpret. This project will use first-principles calculations to simulate spectra from a range of different defects in order to interpret existing experimental data from irradiated samples in terms of structural changes to the material.

60. Modelling the electrocatalytic behaviour of transition metal surfaces.

Robert Weatherup Co-Supervisor(s): Rebecca Nicholls, Jack Swallow

Hydrogen is a promising clean fuel that can be produced using renewable energy by the electrochemical splitting of water. To produce hydrogen efficiently, electrocatalysts are used to increase the reaction rate. Platinum is the catalyst material of choice for the hydrogen evolution reaction, exhibiting small overpotentials at a given current density compared to other transition metals. However, Pt is very expensive and scarce making the high catalyst cost a barrier to commercial uptake of hydrogen production by water splitting.

In this project we aim to employ density functional theory calculations to study the reactivity of metal surfaces with hydrogen with the aim to better understand their catalytic properties. These may be directly compared to that of Pt with the view to find cheaper alternatives without large reductions in performance. We intend to study the surface energetics of a number of abundant metals (e.g. Cu, Ni, Co, Fe, etc.) in the presence of molecular hydrogen to screen which (if any) would be viable electrocatalys

61. Understanding the performance of half-metallic ferromagnets at finite temperature

Jonathan Yates Co-Supervisor(s): Chris Patrick

Some materials with the formula Co_2XZ (X = transition metal, Z = main group element) are examples of *half-metallic ferromagnets*. Electrons in these materials show either metallic or insulating behaviour depending on their intrinsic spin, which means that the material's electrical properties (e.g. its resistance) can be controlled with a magnetic field. This effect is exploited in giant magnetoresistance (GMR) devices. One of the problems with materials like Co_2XZ is that their half-metallic properties degrade as the temperature increases. In this computational project we will use ideas from statistical mechanics and phonon theory to model half-metallic ferromagnets at finite temperature. This will involve some theoretical work building a model, followed by setting up and running density-functional theory calculations. This project would suit a student interested in using quantum and statistical mechanics to tackle a challenging problem in theoretical modelling.

62. Calculating the evolution of electronic properties from bulk to the nanoscale

Jonathan Yates Co-Supervisor(s): Chris Patrick

The technique of encapsulation — growing materials inside other materials — allows the construction of nanostructures which would be thermodynamically unstable under normal conditions. Such exotic structures are likely to show very different electronic properties compared to their bulk 3D form. This project will use density-functional theory calculations to investigate systematically the effect of reducing the materials from 3D crystals down to the 1D nanostructures formed from encapsulation, and understand the results in terms of established electronic structure theory. It would suit a student comfortable with electronic structure and crystallography, wanting to apply materials modelling methods at the nanoscale.

63. Magnetic coupling across interfaces

Jonathan Yates Co-Supervisor(s): Chris Patrick

Many magnetic devices are built as layered structures, consisting of multiple magnetic and nonmagnetic materials. A key question revolves around how different layers are coupled to each other through the quantum mechanical exchange interaction, especially if they are separated by a nonmagnetic layer.
This project will involve constructing models of these multi-layer interfaces and using state-of-the-art computational techniques to calculate the strength of the exchange interaction. Since some of the software is still undergoing development, the project requires the student to have strong computational skills. An interest in crystallography and magnetic properties would also be helpful.

64. Modelling New Materials for Rechargeable Batteries

Jonathan Yates Co-Supervisor(s): Saiful Islam

Materials performance lies at the heart of the development of green energy technologies such as lithium-ion batteries, and computational methods now play a vital role in modelling and predicting the properties of complex materials. For the rechargeable lithium battery, the positive electrode is one of the major challenges for new electronics and electric vehicles. In addition, there is a growing interest in sodium batteries as the high sodium abundance makes them attractive candidates for low cost grid-storage.

We propose a Part II project using advanced computer modelling techniques to investigate new oxide and oxyfluoride cathode materials for lithium- and sodium-ion batteries. The DFT-based simulations will examine structural, electronic and ion diffusion properties. Overall, we will examine factors that may enhance the energy density and charge/discharge rate of novel battery materials.

Recent Paper on modelling cathodes

Sharpe R, et al., ‘Redox Chemistry and the Role of Trapped Molecular O_2 in Li-Rich Disordered Rocksalt Oxyfluoride Cathodes’, *J. Am. Chem. Soc.* **142**, 21799–21809 (2020)

Review on modelling cathodes

Islam M S and Fisher C A J, ‘Lithium and sodium battery cathode materials: computational insights into voltage, diffusion and nanostructural properties’, *Chem. Soc. Rev.*, **43**, 185-204 (2014) .