DEPARTMENT OF MATERIALS

PART II PROJECTS

2020/2021

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 Tuesday 4th February 2020 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 2020.

The following staff members can be contacted, from 2.30 – 5.00pm (unless otherwise noted) on the same afternoon, either in their office or by phone to discuss the projects listed:

Name	Room	Building	Tel. No.
Dr Natalia Ares	20.09	12/13 Parks Road	73719
Prof David Armstrong	Please contact by email: david.armstrong@materials.ox.ac.uk		73708
Prof. Hazel Assender	30.06	Hume-Rothery Building	73781
Prof. Simon Benjamin	40.02	12/13 Parks Road	73732
Prof. Harish Bhaskaran	40.21	Engineering & Technology Bldg	73772
Dr Sebastian Bonilla	Available to meet w/c 17th Feb – please email to arrange: sebastian.bonilla@materials.ox.ac.uk See also note under Peter Wilshaw		83214
Prof Andrew Briggs	30.05	12/13 Parks Road	73725
Prof. Peter Bruce	10.09	Rex Richards Building	12761
Prof. Nicole Grobert	Available to meet on 7th February – please email to arrange: nicole.grobert@materials.ox.ac.uk		83720
Prof. Chris Grovenor	50.12	Engineering & Technology Bldg	73751
Prof. Angus Kirkland	Please contact by email: angus.kirkland@materials.ox.ac.uk		73662
Prof. Sergio Lozano-Perez	30.06	Holder Building	73795
Prof. James Marrow	10.18	21 Banbury Road	73938
Prof. Michael Moody	30.20	Hume-Rothery Building	73693
Prof. Peter Nellist	30.05	Holder Building	73656
Dr Rebecca Nicholls	30.10	Holder Building Only available until 3.45 pm	73707
Prof Mauro Pasta	40.29	Rex Richards Building	12991
Dr Alex Robertson	10.01	14 Parks Road	12993
Prof. Jason Smith	30.10	12/13 Parks Road	73780
Prof. Susie Speller	20.05	21 Banbury Road	73734
Prof. Richard Todd	40.23	Engineering & Technology Bldg	73718
Prof. Andrew Watt	10.45	Begbroke Science Park	13456
Prof. Rob Weatherup	30.09	12/13 Parks Road	73724
Prof. Angus Wilkinson	10.19	21 Banbury Road	73792
Prof. Peter Wilshaw	Currently unavailable but interested students may visit the semiconductors lab (ETB 30.19) and have a chat to Poppy and Alex regarding what the projects involve and the lab environment.		
Prof. Jonathan Yates	20.03	15 Parks Road	12797
Prof. Neil Young	30.10	Holder Building	73655

PROJECTS ON OFFER:

Microwave probing of mechanical motion

Natalia Ares Co-Supervisor(s): Andrew Briggs

Microwave cavities allow us to gain exquisite control of the vibrations of very thin membranes. The aim of this project is to optimize the interaction of microwave photons in a cavity with the motion of nanometer-thick membranes with the goal of exploring quantum motion, amplification and sensing. The project is likely to be of interest to those students that enjoy exploring microwaves circuits and nanoscale motion.

Superconducting resonators for quantum device readout

Natalia Ares Co-Supervisor(s): Susie Speller, Andrew Briggs

Thin-film superconductors can be used to fabricate electromagnetic cavities. By trapping photons, they allow for very sensitive probing of nanoscale devices. The aim of this project is to fabricate and characterize a superconducting radio-frequency cavity with a tuneable frequency. Such a cavity would be key for the readout of spin states in quantum devices and detecting the displacement of nanomechanical resonators. Students that are keen on nanofabrication and the superconducting properties of materials will find this project particularly exciting.

Software development for quantum experiments

Natalia Ares Co-Supervisor(s): Andrew Briggs

Quantum experiments require the control of a variety of electrical signals with precise timing. This project aims at expanding the capabilities of Pygor, a software package that we have created to efficiently interface with quantum experiments. We want to develop the control of high frequency pulses. The project is likely to be of interest to those students that enjoy programming and machine learning, and who are excited about quantum technologies.

Mechanical Testing of Novel High-Entropy Alloys for Nuclear Application

David Armstrong Co-Supervisor(s): Bo-shiuan Li

High-entropy alloys (HEAs) are a novel class of alloys developed in the early 2000s which do not contain a major constituent metallic element (usually three to five equiatomic elements). Due to its high configuration entropy and severe lattice distortion, HEAs possess outstanding mechanical performance even under extreme nuclear environment. This project will utilise high-temperature macro-mechanical testing techniques (fourpoint bending, compression, up to 600 °C and digital image correlation) and room temperature micro-mechanical testing on several novel refractory HEAs developed and manufactured in Oxford. Scanning electron microscopy techniques (EDX, EBSD) will be used to systematically characterise both microstructure and deformations (slip, twinning, fracture) as a function of temperature. Outcomes of the mechanical testing/characterisation will be used to provide manufacturing guidelines for the alloy processing group in Oxford. This project will work alongside micro-mechanical testing of the same materials. Strong interactions will be made with both UK/USA collaborating universities.

Mechanical properties of solid state lithium ion batteries

David Armstrong Co-Supervisor(s): Ed Darnbrough

The ceramic lithium ion conductor Li7La3Zr2O12 (LLZO) has been shown to be promising electrolyte materials for solid state lithium ion batteries. While its electrochemical properties have been well studied there is comparatively little information on the mechanical properties of these materials. This data is a key requirement for the development of a better model of the mechanical behaviour of the materials during the charge-discharge cycle. 10 This project will use a range of nano and mico-mechanical indentation methods to study, the hardness, elastic modulus, yield stress and fracture toughness of these materials processed in both bulk and thin film forms. These properties will be related to local microstructural features through the use of scanning electron microscopy (SEM), Electron back scattered diffraction (EBSD) and Raman Spectroscopy. Finally these micromechanical properties will be compared to bulk fracture properties obtained through four point bend flexure tests. The data produced in this way will not only be useful for seeding models but allow optimisation of processing routes for producing electrolytes with improved lifetimes.

Nanostructured nickel alloys for molten salt cooled reactors

David Armstrong Co-Supervisor(s): Chris Grovenor

Next generation nuclear fission plants will require materials able to operate in more extreme environments. Nickel alloys containing oxide particles are being developed for use in molten salt cooled reactors. These materials contain oxide particles to “capture” and “store” the helium produced during transmutation of the nickel. How this effects the mechanical properties is not well understood. This project will use helium ion implantation to introduce 2000 appm of helium into ODS and non ODS containing materials. These samples will be studied with high speed nanoindentation allowing large maps (upto 1 million indents) of mechanical properties to be constructed. Electron microscopy (SEM EDX and EBSD though TEM maybe possible) will be used to correlate the mechanical properties with helium bubbles, grain structures, ODS particle locations and other mechanical properties.

Zirconium alloys for Fusion

David Armstrong Co-Supervisor(s): Chris Grovenor

Zirconium alloys are being considered for applications in the breeder blanket assembly of new fusion reactor designs, but the current ZrNb alloys used in fission reactors cannot operate above 350oC. The Zr-V binary system has a very similar phase diagram to Zr-Nb but about 200oC higher, and this project will investigate the physical metallurgy, and liquid metal corrosion resistance of dilute alloys fabricated by arc melting using SEM, XRD and hardness measurements to explore the potential of this alloy system (an other Zr-BCC systems such as Zr-Mo) for high temperature applications.

Effects of hydrogen on mechanical properties of palladium

David Armstrong Co-Supervisor(s): Angus Wilkinson

Palladium is a leading metal to play a major role in virtually every aspect of a future hydrogen economy, including purification, storage, detection, and fuel cells. Palladium has the ability to take up large quantities of hydrogen at room temperature and pressure, and subsequently forms palladium hydride (PdH_x). This reversible and the hydrogen can be subsequently extracted. The effects of this on the mechanical properties of palladium is not well understood.

This project will use nanoindentation, AFM and scanning electron microscopy to study the deformation mechanical in virgin and hydrogen containing palladium.

Characterization of gas-barrier polymer films

Hazel Assender

The wider exploitation of flexible functional materials can be limited by the performance of transparent flexible gas barrier materials to exclude water vapour from sensitive device materials. Recent work has cast doubt on the previous understanding of the dependance of water permeation on temperature and humidity and this project seeks to clarify this issue by extending the partial data published to date and hence clarify the underlying mechanism of permeation.

Evaporated molecular semiconductors for flexible electronics

Hazel Assender

Molecular semiconductors can be evaporated for flexible electronics e.g. OTFTs. Much research has focused on very slowly evaporated materials. This project will explore the impact of deposition conditions on the structure and electronic properties of molecular semiconductors. This will include vacuum level, residual gas, deposition rate, and directed ‘vapour jet’ evaporation for creating selective area deposition, and consideration will be made of changes in performance as the deposited materials age.

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 reative centres (radicals) with the nature of the cross-linked network.

Predicting the pervormance and usefulness of near-term quantum computers

Simon Benjamin

Quantum computer prototypes are reaching the point that they are interesting beyond being physics experiments – for example, in 2019 Google announced a 53 qubit device, which is sufficiently large that no conventional computer can predict its behaviour. However, the question of whether such a machine can be useful for anything is still undecided; because each elementary operation, or 'gate' in the machine is imperfect, with up to 1% noise, the output after many gate operations is very noisy and imperfect. All such devices are called NISQ for Noisy Intermediate Scale Quantum systems.

In order to investigate ways in which such machines can be harnessed, it is valuable to have emulator software – this is software that runs on a conventional computer and accurately models how a quantum computer would behave, including any noise processes. The costs in terms of memory (RAM) and runtime rapidly become impractical as the number of qubits rises past 40, but there is much to be learned by emulating even small systems.

The project will include these themes:

- Understand the key concepts of how we use software to emulate quantum computers (especially the QuEST system that uses either Mathematica or c code as the user interface, and ProjectQ that uses python)
- Understand how quantum algorithms are believed to be superior to conventional algorithms for tasks like predicting the properties of novel materials or chemicals.
- The main part: Investigate whether these quantum algorithms can really work on near-future quantum hardware that suffers from imperfections in all operations
    - In tackling this, it will likely be useful to talk to experimental teams, both in Oxford and elsewhere, so as to understand the particular problems their prototype hardware has and thus emulate those problems accurately.

This project will involve a considerable amount of computer programming, and will suit a student who has previous programming experience and enjoys that kind of task.

Novel materials research for photonic computing based AI and/or artificial retinas

Harish Bhaskaran

Project description to follow

EHD printing projects for additive nanomaufacturing

Harish Bhaskaran

Project description to follow

Tunnelling in ion-doped oxide thin films

Sebastian Bonilla Co-Supervisor(s): Peter Wilshaw

This project aims to study the effects of ion doping in the tunnelling current densities across 1-2 nm thin SiO2 dielectric films. It will involve establishing a reproducible and controllable method of growing nanometre scale thin oxides using rapid thermal annealing and nitric acid oxidation, followed by thermal evaporation of metal contacts, accurate IV probing, and temperature variation experiments. After the methodology is stablished and compared to literature works, the addition of alkali cations to the grown SiO2 films will be evaluated to establish the changes in charge transport mechanisms across such ultra-thin oxides. The 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 silicon oxide films will be employed in the next generation of silicon solar cells to produced metal-semiconductor contacts 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.

Electrostatic doping of graphene monolayers

Sebastian Bonilla Co-Supervisor(s): Peter Wilshaw

This project aims to demonstrate the control of charge carrier concentration in graphene as a result of electrostatic charge in a neighbouring dielectric thin film. It involves transfer of CVD graphene onto specially designed dielectric substrates, which have a pre-arranged metal electrode configuration, and can be deposited/embedded with a concentration of static charge. The created devices will be measured to test sheet resistance and hall mobility, as a function of dielectric charge concentration. This project requires hands-on electrical and optical measurements of materials, as well as data processing and analysis. Demonstrating highly conductive graphene as a results of a charged dielectric can enable its use as a transparent conductor in flexible electronics and tandem solar cells. The production of such devices is, as of yet, limited by the lack of a suitable transparent electrode.

Exploring new insights into the Si-SiO2 interface physics

Sebastian Bonilla Co-Supervisor(s): Peter Wilshaw

The Si-SiO2 interface is undoubtedly one of the best studied and understood interfaces used in electronic devices today. However, recent work at Oxford has shown that electrical characteristics of this interface cannot be fully explained by the currently established models of charge dynamics. This project aims to shed light into these unexplained observations, via a combination of experiments and modelling work. It will involve measuring electrical properties of the interface using established techniques like admittance spectroscopy, XPS, and DLTS, and revising the current models that describe the physics of this interface to account for new observations. This project is best suited for someone keen to write Matlab code, explore different modelling approaches, and develop software analysis routines. The Si-SiO2 interface is not only of importance for microchips, but it is the sole responsible in minimizing surface losses in silicon solar cells. The understanding from this project can result in improve processing of commercial solar panels.

Nanomaterials for Thermal Management in Electronics

Nicole Grobert

The continuing trend of electronics miniaturisation is coupled with increased power density of devices, which thereby release significant amounts of thermal energy as waste. Thus, a challenge exists for this generated heat to be dissipated rapidly from devices to the ambient. This project will explore the use of hybrid boron nitride and carbon nanomaterials for use in thermal management materials and/or potting materials along with polymer matrices. When combined, these nanomaterial fillers may display emergent complementary effects on enhancing thermal conductivity, reducing electronic conductivity and enhancing the polymer composite mechanical strength.

Aerogel synthesis towards targeted applications

Nicole Grobert

Aerogels are a diverse class of porous solid materials. The advantage of aerogels lies in their low density. Synthesis parameters are key to control their porosity and the overall properties of the final aerogel. This project is exploratory and will exploit existing techniques developed by the Nanomaterials by Design team and develop new methods towards aerogels containing nanomaterials. Carbon and non-carbon based nanomaterials will be used to generate aerogels that will then be characterised and their properties will be evaluated with view to a series of applications.

Development of the blow spinning technique for eco-friendly (magnetic) polymer fibre fabrication

Nicole Grobert

The blow spinning is a facile and inexpensive technique for polymer fibre fabrication. The main aim of the project is to use the blow spinning set up and test several polymers dispersed in eco-friendly solvents. The basic characterisation tools will be used to estimate the quality and morphology of the fabricated fibres. The produced fibres can be potentially applied in in various fields of science including biomedicine as well as micro/nano engineering.

Time permitting this project will also explore routes to the fabrication of magnetic polymer fibres using the blow spinning technique.

Production and mechanical testing of hierarchical composite structures by freeze casting for energy, thermal, or structural applications

Nicole Grobert Co-Supervisor(s): Richard Todd

Freeze casting is a simple but efficient technique that can help to overcome these challenges. The project concerns the controlled production of hierarchical structures consisting of aligned structural features through the freeze casting of suspensions containing nanomaterials. The aim of the project is to understand the effect of different parameters in order to produce structures providing particular functional or structural advantages. Examples include the production of materials with anisotropic thermal conductivity for thermal management in silicon devices, high surface areas for catalysis, continuous phases for solid state battery electrolytes or as scaffolds for drug testing.

Carbon fibre laminate…. Full title tba

Nicole Grobert Co-Supervisor(s): Roger Reed

Carbon fibre laminate (CFL) composite materials are an established technology frequently applied in the motor or spacecraft industries where thermal management is crucial. Example applications include housing of electronic instrumentation and batteries. Whilst the overall nature of CFLs are interesting, in principle, for telecommunication applications, too, they are non-transparent to radiofrequencies and hence unsuitable. This projects will explore the design, fabrication, and testing of carbon fibre laminate equivalents that are free of carbon fibres and that can be tuned to transmit specific radio frequency ranges. This project is likely to involve engagement with industry partners.

The effect of nitrogen on the properties of thin film solid state electrolytes

Chris Grovenor Co-Supervisor(s): Susie Speller

Thin film sold state batteries are exciting a lot of interest to replace normal Li-ion batteries containing liquid electrolytes that are heavy and have shown some significant safety problems. This project will use sputtering to control the N content of thin films of different electrolyte compounds (including LiAlGePO and LiLaZrO compounds we are already working on) to explore the interesting possibility that the ionic conductivity can be improved by making oxy-nitride materials by distorting the ionic lattice. The project will involve film growth, careful characterisation by SEM/XRD and electrochemical testing.

Joints in practical superconductors

Chris Grovenor Co-Supervisor(s): Susie Speller

The large magnets required for applications in medical MRI and large physics experiments like the LHC at CERN are all based on superconductors and contain numerous joints that are often the (very expensive) points of failure. This project will work with our industrial colleagues on the materials science aspects of making and testing joints in superconductor wires and tapes – how to improve reliability and performance, and understanding what goes wrong. The project will involve designing joint making processes, using XRD and analytical SEM to check phase purity and distributions in the joints, and high current measurements.

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.

Atomic resolution electric field mapping

Angus Kirkland

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.

Optimizing SIMS mapping of nuclear materials

Sergio Lozano-Perez

This project aims to provide with a comparative study of the lateral and mass resolution between the NanoSIMS and the FIB-SIMS. A selection of materials from the nuclear industry (e.g. Zr-alloys for fuel cladding and austenitic alloys from the primary circuit) will be used to better understand the advantages and disadvantages of both approaches and how to optimise them. There is potential for 3D characterisation. The student will become familiar with all aspects of data acquisition and analysis.

In situ Study of Damage in Carbon-Carbon Composites for Gen IV Nuclear Energy

James Marrow

Carbon-fibre/carbon matrix (C-C) composites are proposed for structural components (e.g. control rods, heat-exchangers) in next generation high temperature nuclear fission reactors.

To select materials and fabrication methods that will contribute to long and economical reactor lifetimes, it is important to be able to assess the effects on the material of exposure to the reactor environment (high temperatures, coolant and irradiation). Assessing and qualifying such environmental effects using Materials Test Reactors requires the testing of small specimens, for which suitable methods do not exist. Novel methods to analyse damage small specimens, based on analysis of crack fields, have been developed in Oxford (https://doi.org/10.1016/j.ceramint.2019.06.016, https://ora.ox.ac.uk/objects/pubs:610901), and these aim to provide the inputs for multi-scale modelling of composites.

In this project, in collaboration with ANSTO (Australian Nuclear Science and Technology Organisation) you will use in situ testing and digital image correlation of optical data and three-dimensional X-ray tomographs to examine fracture nucleation and propagation in C-C composites from the Generation IV International Forum (GIF) programme. The project asks the question "What are the criteria for crack initiation and propagation in C-C composites, and how are they affected by microstructure?". The project will involve mechanical testing, computed tomography, data visualisation and numerical analysis (Matlab), with opportunities to apply finite element simulation.

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

James Marrow

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 with mechanical properties and electrical properties that are enhanced by CNT networks, self-entangled around a highly porous 3D ceramic ’tetrapod’ foam (https://doi.org/10.1038/s41467-017-02372-9). It has an open structure with a high porosity and pores in the range of several μm, which is beneficial for several applications due to high surface accessibility.

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 an experiment to study the compressive and tensile 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.

Atom Probe and Digital Field Ion Microscopy for Combined Atomic-Scale Structure and Chemistry

Michael Moody Co-Supervisor(s): Paul Bagot

Whilst atom probe tomography (APT) is unsurpassed at routinely providing 3D chemical information at the atomic-scale, its spatial resolution is not sufficient to observe the underlying crystal structure. In contrast, its predecessor, field ion microscopy (FIM) has poor chemical resolution, but 2D spatial resolution not only capable of imaging the crystal but also of directly identifying lattice defects down to the level of individual vacancies.

This project will develop applications of the digital FIM capabilities in the recently installed LEAP 5000 XR. APT and FIM will be combined to investigate atomic-scale chemistry and structure of features such as the formation of precipitates in heat-treated alloys and microstructural damage induced by irradiation in materials for fission and fusion reactors.

Characterising Atomic-Scale Microstructure in Alloys Designed for Fission and Fusion Reactors

Michael Moody Co-Supervisor(s): David Armstrong and Paul Bagot

Many materials for safety critical components to withstand the extreme environments fusion and fission reactors must be designed at the atomic-scale. Hence high resolution characterisation is a critical step in alloy design and the development of processing routes to optimise these materials. In the Materials Department we are developing high entropy alloys for fusion reactors and nanostructured nickel based ODS alloys for molten salt fission reactors.

In this project, 3D nanoscale atom probe tomography analyses will be used to characterise the new materials and inform the next iteratiion of processing steps.

Controllable deployment of next-generation Li-ion cathode materials for in-situ transmission electron microscopy

Alex Robertson Co-Supervisor(s): Peter Bruce

Understanding how new electrode materials for rechargeable batteries evolve and degrade under application-relevant conditions provides us the information necessary to tailor the material to be more robust, providing longer-life and more economic batteries. One of the best techniques for understanding nanoscale structure is the TEM, but the vacuum of the TEM is mutually exclusive with the liquid electrochemical environment practical Li-ion batteries require. To image electrodes in-situ, inside a liquid electrolyte while also being electrically cycled, requires advanced microelectromechanical (MEMS) chips to encapsulate the micron-scale electrochemical cell in a way that is compatible with simultaneous TEM imaging.
A major challenge in exploiting this technique is anchoring novel electrode materials to the silicon MEMS chips.

This project will tackle this challenge, developing and implementing a route for controllable anchoring of electrode materials of interest to in-situ TEM MEMS chips. The student will prepare a composite electrode material – metal oxide nanoparticle electrode materials ensconced in a carbon nanotube conductive web – that is amenable to electrophoretic deposition to the target silicon MEMS devices. Following the development of a consistent technique for reliably anchoring the composite to the MEMS devices, the student will collaborate with group members to perform advanced in-situ liquid electrochemical TEM studies of the prepared electrodes, revealing the nanoscale structural evolution of next-generation Li-ion metal oxide cathodes. The student will gain skills in nanomaterial synthesis and SEM/TEM characterisation, electrochemistry, electrophoresis, electrical measurement of nanodevices, and ultraviolet lithography for device fabrication.

Measurement 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 involve the construction of a new device to detect UFPs using single photon detection methods. The aim is to demonstrate a device that can measure particle concentrations as low as 1000 per cubic centimetre that could be adapted for use in public spaces.

Laser-written defects in wide band gap crystals for quantum technologies

Jason Smith

Fluorescent point defects (aka colour centres) in wide band gap crystals are attractive as qubits in future quantum computers. We have shown recently that laser processing with focused sub-picosecond pulse can be used to engineer defects in diamond on length scales as short as 50 nm providing a potential manufacturing route for chip-scale devices. Several other materials besides diamond, such as SiC, GaN, and ZnO, are also beginning to attract significant attention. This project will involve writing and characterising colour centres in such materials using laser processing methods, and evaluating of their optical and spin properties for use in quantum technologies.

Quantum gates using engineered nitrogen-vacancy defects in diamond

Jason Smith

The electronic spin state of NV defects in diamond is a front-runner qubit for quantum computing, with the promise of chip-scale device that are robust to imperfections by virtue of a networked architecture. The goal of this project is to perform logical gate operations on engineered NV qubits in diamond membranes and measure the gate speed and degree of precision (fidelity) that can be achieved. You will work within a wider team developing engineered materials and devices for diamond quantum computing, and within the UK Hub in Quantum Computing and Simulation.

High temperature superconducting thin films to test ideal joint performance

Susie Speller Co-Supervisor(s): Chris Grovenor

The large magnets required for applications in medical MRI and large physics experiments like the LHC at CERN are all based on superconductors and contain numerous joints that are often the (very expensive) points of failure. Understanding the properties of joints between commercial wires and tapes is complicated by their 3D structure and polyphase nature, and this project will fabricate thin films of Gd1Ba2Cu3O7 and use these 'ideal' surfaces to fabricate and test joints to identify the fundamental limits of performance we can then aim for in practical joints between real superconductors.

Superconducting properties of MgB2 bulk magnet materials

Susie Speller Co-Supervisor(s): Chris Grovenor

Magnesium diboride is an interesting superconducting material for applications in high field permanent magnets for small medical MRI machines. We are working with external collaborators to develop these magnet materials, including Element6 who use 6 GPa hot pressing to give unique microstructures. This project will use XRD and SEM, and electrical measurements at cryogenic temperatures, to study samples processed under a range of different conditions to understand the relationship between microstructure and properties. If the student was keen, the project could have a component on the modelling of trapped field.

Processing of electrolytes for solid state batteries

Richard Todd Co-Supervisor(s): Mauro Pasta

Solid state Li batteries should, in principle, possess better specific power capacity and be safer than existing Li-ion batteries. However, problems are experienced with the formation of Li dendrites in the solid-state electrolytes used. Most work so far has used discs processed using the most basic of ceramic processing methods. Better processing and more refined geometries should alleviate the dendrite problem. This project will investigate the processing of doped LLZO (Li7La3Zr2O12) ceramics to obtain high density and flexible geometries.

Quantum Dot Solar Cells

Andrew Watt

Solar cells based on lead sulfide colloidal quantum dots as the absorber have the potential to provide cheap, flexible, and highly efficient photovoltaic devices. Lead and sulfur are both abundant, low-cost materials that can be synthesized into nanocrystal colloids which absorb across the solar spectrum. These colloids can be solution-processed into thin films with controlled semiconductor properties suitable for optoelectronic devices. Since the first report of a Schottky junction solar cell in 2005, power conversion efficiencies (PCE) have increased from less than 1% to 11.3%.

During this Part II project you will learn how to synthesise quantum dots. fabricate solar cells and characterise their properties. A range of techniques including electron microscopy and optoelectronic characterisation will be used along with opportunities to learn instrumentation control using LabView or Matlab.

References

Neo, D. C. J.; Cheng, C.; Stranks, S. D.; Fairclough, S. M.; Kim, J. S.; Kirkland, A. I.; Smith, J. M.; Snaith, H. J.; Assender, H. E.; Watt, A. A. R. Influence of Shell Thickness and Surface Passivation on PbS/CdS Core/Shell Colloidal Quantum Dot Solar Cells Chem. Mater. 2014, 26 (13) 4004– 4013DOI: 10.1021/cm501595u

Zhang, N.; Neo, D. C. J.; Tazawa, Y.; Li, X.; Assender, H. E.; Compton, R. G.; Watt, A. A. R. Narrow Band Gap Lead Sulfide Hole Transport Layers for Quantum Dot Photovoltaics. ACS Appl. Mater. Interfaces 2016, 8 (33), 21417– 21422, DOI: 10.1021/acsami.6b01018.

Solvodynamic Printing of Nanowire Networks

Andrew Watt

The patterning of functional materials has become an important aspect of manufacturing technology as it is essential in the fabrication of devices like microelectronic integrated circuits, microelectromechanical systems, optoelectronic devices and DNA microassays. Traditionally, high resolution patterning is done via lithographic techniques which can achieve resolutions in the nanometer range.

However, such techniques are usually multi-step, require expensive equipment and low in throughput. As a result, additive ink-based printing techniques like inkjet, flexographic and gravure printing have become increasingly used and sparked the development of the field of printed electronics. Such techniques have substantially lower costs and are compatible with large area high throughput processes.
In this Part II project you will use solvent-solvent interactions to create high resolution features for printed electronic applications using additive patterning techniques and nanowire colloids. A range of techniques including electron microscopy and electronic characterisation will be used along with opportunities to learn instrumentation control using LabView or Matlab and the integration of materials produced in to solar cell devices.

References

Solvodynamic Printing As A High Resolution Printing Method WC Liu, AAR Watt, Scientific reports 9 (1), 1-12 2019.

Thin film deposition of battery cathode materials

Rob Weatherup Co-Supervisor(s): Susie Speller

Future generations of Li-ion batteries for electric vehicles, require further improvements in energy density which is primarily limited by the cathode (positive electrode) materials currently used.

This project will apply pulsed laser deposition to grow thin films of mixed transition metal oxides as high-capacity cathode materials for Li-ion batteries (e.g. Nickel-rich Lithium Nickel Manganese Cobalt Oxides). Different methods to control chemical composition will be investigated, such as deposition from mixed oxide targets and multilayer deposition from multiple targets. These films will be characterised using XRD, SEM and XPS, and the performance of the different materials confirmed through the assembly and electrochemical testing of Li-ion cells (Galvanostatic cycling and impedance spectroscopy). By growing these films on thin (<100 nm) silicon nitride windows, it will then be possible to perform operando X-ray spectroscopy measurements during charging and discharging at synchrotron facilities such as Diamond, and to perform TEM characterisation of the cycled films.

Atomically clean 2D material membranes for photoelectron spectroscopy of solid-liquid interfaces

Rob Weatherup

XPS 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/hexagonal boron nitride) 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 the development of methods to cleanly transfer and suspend them over perforated supports. These suspended membranes 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 at the graphene interface under electrochemical bias using lab-based XPS systems in the department. This may then be extended to time- and depth-resolved measurements using synchrotron facilities such as Diamond Light Source.

Corrosion protection with 2D materials

Rob Weatherup

Graphene and other two-dimensional (2D) materials offer the prospect of preserving the physical properties of surfaces with only a single atomic layer separating them from their surroundings. When these 2D materials are grown by chemical vapour deposition (CVD) on certain substrates, a strong interaction is established which oxidation of the surface even after during extended air exposures. However the CVD process requires high temperatures where atomic diffusion is significant, making it unsuitable for direct interaction with the nanometre-sized features present in many electronic devices.

This project aims to develop a new low-temperature approach for establishing a strong interaction between transferred 2D materials (graphene and hexagonal boron nitride) and a substrate.

This will enable the integration of 2D materials with delicate magnetic structures such as Co-Pt multilayers that cannot survive typical CVD temperatures. You will develop methods for reliably transferring 2D materials, and use approaches such as vacuum annealing to establish a strong interaction with the substrate. XPS and SEM will be used to investigate how effectively these surfaces are protected from oxidation, and confirm whether Co-Pt multilayer structures are preserved. These protected multilayers will then be integrated into spintronic devices with involvement of collaborators in Paris.

Alternatively, the project could focus on low cost methods for protecting metals from corrosion in aqueous environments, where anchoring of the edges of exfoliated 2D material flakes to the metal by chemical modification might be explored.

Revealing the impact of vibrations on degradation in lithium ion batteries

Rob Weatherup

Lithium ion batteries (LIBs) are increasingly used in portable electronics and electric vehicles. Much research has focussed on identifying the degradation processes taking place in LIBs in order to extend their working life and decrease the frequency of replacements. This has mostly considered cells that aren’t subjected to mechanical stresses, whereas in real applications there is often significant vibration which may influence battery performace.

This project will apply controlled vibrations to LIBs whilst they are charged and discharged and use surface characterisation techniques to reveal how the electrode surfaces are affected by the vibrations and correlate these findings with the electrochemical performance of the cells. The surface characterisation will include x-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), as well as advanced and synchrotron based techniques such as X-ray Absoprtion Spectroscopy (XAS).

High Entropy Alloys for nuclear application

Angus Wilkinson Co-Supervisor(s): David Armstrong and Bo-shiuan Li

The so-called high-entropy alloys (HEAs) are a novel class of alloys developed in the early 2000s which do not contain a single major constituent metallic element, but instead have 4-5 elements at similar high concentration. Although the early hypothesis that high configurational entropy might act to stabilise a single phase in such systems has generally been rejected, research has stimulated activity that has revealed a rich seam of novel highly alloyed metallic that possess outstanding mechanical performance.

Of particular interest for nuclear applications are a series of low activation refractory alloys which we have shown to exhibit remarkably little hardening due to irradiation. This project will continue development of these alloys and their heat treatment schedules using arc melted billets. Processing-microstructure relationships will be explored using a variety of modern methods including XRD, SEM, EDX, EBSD, TKD as appropriate. Mechanical properties will be assessed with nanoindentation, micro- and macro- scale mechanical testing including at elevated temperatures.

Ultrasonic Fatigue testing

Angus Wilkinson Co-Supervisor(s): Jicheng Gong

Fatigue is a dominant failure mode in service and is pervasive across industrial sectors. In the (very) high cycle fatigue (V)HCF regime initiation (ie nucleation of a physical crack and its growth to an engineering relevant defect) dominates the fatigue lifetime. We have developed an ultrasonic testing method that allows rapid testing (at 20 kHz 106 cycles in 50 secs) of small test volumes (~100 μm across). Most recently we have produced a rig enabling testing in situ in our Zeiss Merlin FEG-SEM. Cycling is too rapid for dynamic observation but imaging the evolution of the sample after blocks of loading cycles is readily accomplished.

This project will focus on austenitic stainless steel and explore the use of this rig combined with HR-DIC and HR-EBSD mapping of the sample to characterize local deformation evolution that eventually leads to the nucleation of a fatigue crack.

Advancing Phase Identification from EBSD Patterns

Angus Wilkinson

Automated analysis of EBSD patterns has led to an incredibly powerful materials characterization method that generates detailed maps of crystal orientation, misorientation, lattice strain and dislocation content. Analysing crystal phases however is limited to distinguishing between best matches of candidate crystals that have already been identified and recorded in a database. A huge drawback is that if a crystal is not in the database then it cannot ever be found.

This project aims to implement a very different approach using image analysis methods to search for symmetry elements present in the patterns and from this build up a description of the crystal geometry from first principles. We will develop from ideas described in [1] but using image analysis methods to automate the process, and working towards new functionality within the open source AstroEBSD Matlab code [2].

[1] Dingley and Wright, J Applied Crystallography (2009) 42, 234-241, https://doi.org/10.1107/S0021889809001654

[2] Britton et al, J Applied Crystallography (2018) 51, 1525-1534, https://doi.org/10.1107/S1600576718010373.

Metal-metal asperity contact: Understanding fundamentals of wear

Angus Wilkinson Co-Supervisor(s): Anna Kareer

Wear of materials is a complex phenomenon that is not fully understood. The development of instrumented indentation systems (nanoindenters) has provided a platform with which the contact of single asperities can be isolated and studied in well-controlled experiments. Almost all nanoindentation studies use a hard diamond indenter tip to probe a softer flat polished sample surface. This project will make a significant change by exploring metal – metal contacts. During indentation testing it is likely that significant deformation will occur in the tip as this is less constrained than the substrate. The engineering and science challenges include designing and making our own metallic tips to mount in the nano-indenter, understanding how tip shape evolves, understanding how the tip material work-hardens, understanding adhesion to substrate as the tip is retracted, and any material transfer that takes place.

Nanoscratch testing: Understanding fundamentals of wear

Angus Wilkinson Co-Supervisor(s): Anna Kareer

Wear of materials is a complex phenomenon that is not fully understood. The development of instrumented indentation systems (nanoindenters) has provided a platform with which the contact of single asperities can be isolated and studied in well-controlled experiments. Nanoscratches can be formed by making an indent and then translating the sample whilst the indenter loading is maintained. Nanoscratches have been less extensively studied than nanoindents.

This project will undertake nanoscratch experiments on polycrystalline Fe and Fe-Cr (BCC) samples. The effects of Cr content, crystal orientation within a grain, and grain boundary character, on the scratch response will be investigated. EBSD, SEM and AFM will be used to study the scratch track as it crosses the grain boundary and proceeds into the next grain with different crystallographic orientation.

Neighbourhood effects in deformation of Ti alloys

Angus Wilkinson Co-Supervisor(s): Ed Tarleton

The hcp crystal structure of alpha-Ti alloys leads to some grain orientations that are very hard (c-axis parallel to load axis) compared to others which are relatively soft under uniaxial loading. This leads to quite marked grain-to-grain differences in the stress and strain levels which depart strongly from the sample averaged values. Furthermore, the critical resolved shear strength of <c+a> slip is known to be stronger in compression than in tension.

This project will explore how this tension-compression asymmetry affects the distribution of stress and strain at the grain level for uniaxial tension and compression test. If time allows we may also look at cyclic deformation. A combination of digital image correlation, HR-EBSD, and/or crystal plasticity FEA simulations will be used. This follows a previous part II study using micro-cantilever bend testing: Roberts, Gong, Wilkinson, Tarleton, Tension–compression asymmetry of 〈c+a〉 slip in Ti–6Al, Scripta Materialia, (2020), 178, 119-123, https://doi.org/10.1016/j.scriptamat.2019.11.002.

Electron microscopy studies of electrochemical transformations

Neil Young Co-Supervisor(s): Richard Compton (Chemistry)

Nanoparticle-based materials enable many technologies where a deeper understanding of material structure-property relations would be desirable. This project will develop techniques for 'ex-situ' TEM studies of electro-chemical transformations, including oxidation and reduction reactions of battery-related nanomaterials and also catalysts. The goal will be to develop methodologies to investigate morphological changes following electrochemical experiments, ultimately leading onto 'in-situ' TEM/electrochemical measurements.

Nanogalvanic reactions studied via TEM

Neil Young Co-Supervisor(s): Richard Compton (Chemistry)

The aim of the project is to investigate galvanic reactions between two different materials while imaged 'in-situ' within the TEM. The project will require you to consider candidate materials for the process, to develop an experimental methodology and to consider the time scales of the reactions that will enable study via TEM. The project is likely to use nanostructured materials such as core-shell particles and ionic liquids, in working towards fully 'in-situ' electrochemical measurements. The project will be split between hands-on characterisation via TEM and electrochemical measurements in the Chemistry Department.

Materials Modelling Laboratory Projects

The following 7 projects all involve electronic structure modelling; either DFT or beyond-DFT methods. They cover a wide variety of materials systems, from battery materials, pharmaceuticals, magnets, to ceramics. All projects involve two supervisors, and we advise talking to both of the supervisors listed on a project you are interested in. However, if you would like to first discuss the modelling projects more generally, please contact Prof Jonathan Yates. Also contact him if you are interested in a modelling project involving a class of material not listed here, as it may be possible to design further projects.

Calculating the magnetrocrystalline anisotropy of cobalt-based magnets

Jonathan Yates Co-Supervisor(s): Chris Patrick

The magnetocrystalline anisotropy (MCA) quantifies a material's preference to have its magnetic moment pointing along particular crystallographic direction, independent of the sample shape. The fundamental origin of the MCA is the spin-orbit interaction, which provides a coupling between the electron spin direction and the crystal axes. The aim of this computational project is to explore two different methods of calculating the MCA within density-functional theory. We will apply the methods to cobalt-based permanent magnets, which have a moderately high MCA. This project would suit a student with strong mathematical and computational skills, interested in studying advanced techniques to model magnetic materials.

Modelling magnets at finite temperature using zero-temperature DFT

Jonathan Yates Co-Supervisor(s): Chris Patrick

Density-functional theory (DFT) calculations of magnetic materials are usually performed on ordered magnetic structures; for instance, where the magnetic moments associated with each atom point in the same direction (ferromagnetic alignment). These structures actually correspond to the magnet at zero temperature. Above T = 0 K, thermal fluctuations will introduce some randomness to the orientation of the individual moments, and above the Curie temperature the moments are completely disordered. In this project we will use statistical methods to go beyond standard DFT calculations and model magnetic materials in this disordered state. By doing this we will be able to calculate the Curie temperature, one of the properties of most interest to researchers looking for new magnetic materials. This computational/theoretical project would suit a student interested in applying statistical mechanics to tackle a challenging problem in computational modelling.

Predicting and understanding the colours of crystals

Jonathan Yates

Many small molecules exhibit the phenomena of polymorphism - the observation that the same molecule can pack together in different ways to form different crystals. This is of major industrial importance, for example pharmaceuticals. Some polymorphs have significantly different optical properties, i.e. their colour. Such molecular crystals have a range of potential applications – inks that can change colour, variable-wavelength lasers, or as a diagnostic tool. The precise conformation of the molecules, as well as the crystal packing, determines the optical properties of the crystal, but a thorough understanding of how is still lacking. This project would use (time-dependent) density functional theory calculations, running on supercomputers, to investigate how the optical properties of such molecules varies with conformation and crystal packing.

Lithium rich anti-perovskite solid-electrolytes for all-solid-state Li-metal batteries

Jonathan Yates Co-Supervisor(s): Mauro Pasta

Rechargeable lithium-ion batteries have revolutionized the portable electronics industry because of their high energy density and efficiency. They may also prove valuable for a variety of other applications, including electrification of the transport system and grid-scale stationary energy storage. However, they still suffer from several significant safety and reliability issues, many of which are related to the use of flammable organic solvents. Solid-state electrolytes could resolve all of these problems. However, most candidate materials have lower ionic conductivity compared to that of liquid electrolytes and are hard to manufacture at scale thus limiting their practical application. Lithium rich anti-perovskites (Li3AX where A = O2-, S2- and X = Cl-, Br-) are considered a promising class of solid electrolytes thanks to their wide electrochemical window, stability in contact with Li metal, high Li-ion conductivity and low melting point in their hydrated form.

This project will use density functional calculations to understand the structure, electronic transport, and Li mobility in these solid electrolytes.

Direct Imaging of Bonding at Atomic Resolution

Jonathan Yates Co-Supervisor(s): Peter Nellist

It is now possible record STEM images which are sensitive to the phase shift of the electron as it passes through the material. The remarkable implication of this is that we can essential look at the redistribution of electrons due to bonding in a material. As well as being a sensitive characterization technique this is a strong test of quantum mechanical approaches such as DFT. This project aims to inform experimental work by computing STEM images of pharmaceutical compounds – addressing one of the grand challenges of polymorphism in pharmaceuticals.

DFT modelling of SiC composites for jet engines

Rebecca Nicholls Co-Supervisor(s): David Armstrong

The interfaces in SiC composites play a key role in the behaviour of these materials. Electron microscopy allows us to collect spectra containing bonding information with atomic resolution. Understanding the spectra is not trivial and this project will use quantum mechanical simulations to interpret them and map how the bonding changes.

DFT modelling of battery materials

Rebecca Nicholls Co-Supervisor(s) Rob Weatherup

The capacities of current generation of Li-ion batteries are primarily limited by the cathode (positive electrode), which is typically based on LiCoO2. There is a strong drive to reduce the Co content of these materials by replacing it with Mn and Ni, which are less toxic, less expensive and can offer higher capacities. However, the increased capacities cannot be fully accounted for by redox process occurring at the transition metal sites, but also appear to involve oxygen redox processes. This project aims to develop density functional theory simulations of O K-edge X-ray absorption spectra that would help determine the O redox processes occurring in these cathode materials. This will help to provide fundamental insights into experimentally observed changes occurring in X-ray absorption spectra that have already been collected at Diamond Light Source. There will also be further opportunities to be involved in synchrotron measurements during the project if desired.