UNDERGRADUATE PART II PROJECTS

The project descriptions can also be found at:
http://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 7 February 2017, with introductory talks on Part II from the Head of Department and the Part II Co-ordinator. Attendance at these talks is mandatory for all MS students commencing Part II in Michaelmas Term 2017.

The following staff members can be contacted, from 2.30 – 5.00 pm (unless otherwise noted) on the same afternoon, either in their office or by phone to discuss the projects listed:
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<th>Name</th>
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<td>Dr David Armstrong</td>
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<td>21 Banbury Road</td>
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<tr>
<td>Prof. Hazel Assender</td>
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<td>Prof. Harish Bhaskaran</td>
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<td>Prof Andrew Briggs</td>
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<td>Prof. Peter Bruce</td>
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<td>Dr Colin Johnson*</td>
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<td>Prof. Edward Laird</td>
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<tr>
<td>Prof. James Marrow</td>
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<td>Dr Jan Mol</td>
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<td>Prof. Mauro Pasta*</td>
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<td>Prof Peter Wilshaw</td>
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*Upon arrival at Rex Richards Building please dial “energy” and you will be met by Zsofia Szabo, Peter Bruce’s PA.

*(Happy to speak to any prospective students by phone or we can arrange a separate time for them to visit Begbroke to see the facilities meet the rest of the people.)

*(only 2-2.30pm – after that time contact Dr Lewys Jones)

*(Samuel Wheeler (samuel.wheeler@queens.ox.ac.uk) will be in Rex Richards to show the laboratory)

*Out of office on 7th Feb, please email: kyriakos.porfyrikis@materials.ox.ac.uk

*(Away on the 7th but will be available in room 40.20 of the ETB at 2pm on Wednesday 8th February.)
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High temperature deformation of geological materials

David Armstrong, Angus Wilkinson

The mechanical behaviour of naturally occurring geological materials such as quartz, olivine or feldspar is important in understanding the macroscopic deformation behaviour of large scale geological structures. However as these crystals typically have large unit cells and low symmetry structures the deformation mechanisms are anisotropic and complex. In particular how these materials deform at high temperatures and over multiple strain rates is not well characterised on a microscopic level. This project will use high temperature micro-hardness testing (up to 1500°C) and nanoindentation to study the effect of temperature and strain rate on both the mechanical strength and active deformation mechanisms in complex geological crystals. High resolution EBSD will be used to measure plastic zone sizes and active slip systems and atomic force microscopy (AFM) and scanning electron microscopy (SEM) will be used to understand fracture behaviour. This project will be in conjunction with Dr David Wallis and Professor Lars Hansen in the Dept. of Earth Sciences.

Characterization of SiC-SiC fiber composite joints for nuclear fuel cladding applications.

David Armstrong, Yevhen Zayachuk, James Marrow

SiC fiber-reinforced SiC matrix composites are suggested for the use as an accident-tolerant fuel (ATF) cladding material for fuel rods in nuclear reactors. Rod end plugs is one of the critical technologies that still need to be developed in SiC-SiC ATF designs. Technologies needed for the gas-tight end-plugs joining will be investigated in collaboration with General Atomics (San Diego, USA).

The aim of the project is to evaluate the efficiency of different joining techniques. In this project you will use mechanical testing - macroscopic fracture and nanoindentation, to compare the properties of the samples made via different manufacturing routes in order to determine which techniques create stronger joining. SEM and X-ray tomography will also be used for investigation their microstructure created by different techniques and for comparison of their characteristic damage mechanisms, in order to correlate fracture properties and material’s microstructure. These measurements will help in the optimization of end-plug manufacturing technology.
Studying Plastic Deformation in Irradiated Nuclear Materials

David Armstrong, Angus Wilkinson, Anna Kareer

BCC metals such as iron, tungsten, vanadium and tantalum are important materials for use in high temperature components in future nuclear fusion reactors, due to their high melting points, and low activations after irradiation. How these materials behave mechanically after irradiation is important for the design of future nuclear reactors, but due to the difficulty of working with neutron irradiated materials most work has focused on using ion irradiation to mimic neutron damage. This damaged layer is typically only a few microns thick so must be studied using nanoscale methods. The Oxford Micro-mechanics group has used nano-indentation to study plastic deformation in irradiated materials, however the effect that irradiation damage has on plastic zone size and shape is not well understood – in particular sub-surface interactions of plastic deformation with the implanted – unimplanted interface which is not easily studied.

Spherical nano-indentation will be used to mechanically load irradiated and unirradiated single grains and grain boundaries in refractory bcc metals. EBSD, AFM and SEM will then be used to characterise the type of grains and grain boundaries being tested and to study the deformation around the indent and at the grain boundary. Ion slicing will be used to produce cross sections and the subsurface deformation at the irradiated/unirradiated boundary studied.

Self assembly of peptides on surfaces

Hazel Assender

Polypeptide sequences can form 3D hydrogels by selective self-assembly depending on the sequence chosen. Collaborators at the university of Manchester (A. Saiani) and a current part II student have been able to cast thin films of these materials with an initial study of how the surface interactions can significantly influence the ordering observed. Such thin film ordering has potential applications in generating surface-directed patterning e.g. for localised biological interactions and nanoscale devices. This project will take forward the study self-assembly behaviour in thin films, including means by which the ordering can be locally tailored for device structures. AFM and other characterisation techniques will be used to study the ordering. These results can be compared with the bulk behaviours observed in Manchester by SANS and TEM.
Characterization of gas-barrier polymer films

Hazel Assender

The wider exploitation of polymer electronics e.g. PV, or flexible displays, is limited by the performance of transparent flexible gas barrier materials to exclude water vapour from the sensitive device materials. The part II project will be focused on manufacture of barrier layers and their characterization by use of the ‘Ca test method’. The microstructure of the features that develop as a thin layer of Ca reacts with water vapour which passes through micro- and nano-scale holes in the barrier material will be observed optically. The technique has opened up a number of questions about the mechanism of gas transport through the layers that this project will seek to explore.

Control of surface chemistry and phase separation in vacuum-deposited acrylate coatings

Hazel Assender

Vacuum deposition of acrylate layers is a novel route to controlled-thickness thin film coatings and membranes. We have started to investigate the deposition of copolymer materials with a mixture of monomers, and this project seeks to explore the control of properties by copolymerization. In particular, the project can explore the partial phase separation of the two monomers prior to polymerization in situ to create multiphase systems. This could have application for surface energy control, for example for tailored biointeractions, or for porous or ion conducting materials. The project will involve deposition of acrylate materials on our semi-industrial scale roll-to-roll facility and characterisation of the resulting properties.

Colloidal lithography using janus particle self assembly

Harish Bhaskaran

Information TBC

Speed of switching of various phase change materials at the nanoscale

Harish Bhaskaran

Information TBC
Inducing quantum interference effects in graphene nanostructures
Andrew Briggs, Jan Mol

Quantum interference effects, like Fano resonances, could be used for low-power electrical switching or highly efficient thermoelectric energy harvesting. Such effects might be induced in graphene nanostructures by chemically doping them with strong acceptor or donor molecules. You will try to test this hypothesis by producing graphene nano-constrictions with a width of only several nm using feedback controlled electroburning. Electrical transport measurements at cryogenic temperatures before and after doping will be used to reveal quantum interference effects.

Measuring the thermopower and the Peltier effect of single molecules
Andrew Briggs, Jan Mol

Thermoelectric effects describe the conversion of temperature gradients into electrical voltages (Seebeck effect) or vice versa (Peltier effect). These effects are very important for future energy harvesting or efficient electrical cooling. You will study the thermoelectric response of a single molecule contacted by graphene nano-electrodes. A microheater and micro-thermocouples close to the junction will be used to create or measure temperature gradients along the device. This allows you to extract the Seebeck and Peltier coefficient of a single molecule.

A graphene based “sniffer dog” for explosives detection
Andrew Briggs, Jan Mol

Detecting explosives sensitively, selectively, rapidly and fault-free is of high importance for civilian security. Most explosives are hard to detect due to their very low vapour pressures and often commercial sensors work only reliable if used close to the analytes and need minutes to detect. Due to their high surface to bulk ratio nanostructures are excellent charge sensors and can enable the fabrication of sensing devices with single-molecule resolution. You will fabricate graphene nano-constrictions by feedback-controlled electroburning and test their electrical response towards different nitro-group containing explosives (TNT, RDX and HMX). Ultimately, you will be able to measure unique electrical fingerprints of explosives to enable selective detection.
3D microwave cavities for sensitive read-out of mechanical motion

Andrew Briggs, Natalia Ares, Edward Laird

Electromagnetic cavities trap photons, which can therefore repeatedly interact with objects being probed. Although the radiation pressure is tiny, it can be harnessed to control moving objects with extraordinary precision.

We are experimentally studying cavities that can trap microwaves to gain exquisite control of the vibrations of very thin silicon nitride membranes. Our laboratory is equipped with state-of-the-art microwave electronics and cryogenic facilities that allow us to reach the quantum regime.

The aim of this project is to optimize the interaction of photons in a 3D microwave cavity with the motion of commercial silicon nitride membranes with the goal of exploring quantum motion, amplification and sensing.

Synthesis and electrochemical characterisation of Na-battery electrode materials

Peter Bruce

The project will involve the syntheis of novel compounds characterisation with XRD, SEM and Electrochemistry. This will be followed by iterative steps to investigate the effect of chemical changes on material performance.

Development of microbatteries for in-situ electrochemistry in the electron microscope

Peter Bruce

The newly available electrochemistry holders for the transmission electron microscope allow imaging in-situ inside the microscope the dynamical changes that happen at the nanoscale in liquid flow cells as charge/discharge cycles are applied, and while simultaneously collecting correlative electrochemical data. In this project, the student will be involved in the development of suitable electrode/solutions that will allow us to reproduce the structure of a lithium, sodium or lithium-air batteries inside the in-situ holder, and to monitor changes upon cycling. Their performance will be compared to that of larger ex-situ cells. The project will require a good understanding of microstructural characterisation techniques and electrochemistry.
Synthesis and electrochemical characterisation of Li-battery electrode materials

Peter Bruce

The project will involve the synthesis of novel compounds characterisation with XRD, SEM and Electrochemistry. This will be followed by iterative steps to investigate the effect of chemical changes on material performance.

Orthodontic device

Jan Czernuszka

This project builds on a TDP on using hydrogels to manipulate the positions of teeth.

Complex interlaced structures formed from natural polymers.

Jan Czernuszka

The project will examine the possibility of using microstructurally controlled structures to help develop a patch following an infarction.

Manufacture of coatings for nuclear power applications

Patrick Grant

Next generation fusion and fission reactors require a combination of neutron irradiation, temperature and corrosion resistance unavailable from current commercial alloys. One of the approaches that has emerged for future materials for use in these environments is to stabilise their microstructural features, such as grain size, with a low fraction but very high number density of stable ceramic nanoparticles, to form oxide dispersion strengthened (ODS) alloys. These particles are also effective in acting as sinks for vacancies and He formed by neutron damage, helping to prolong the alloy's useful lifetime and properties. However, ODS alloys are expensive to manufacture into engineering structures and therefore this project will explore the feasibility of applying ultra-thick (1 mm) ODS alloy coatings, using vacuum plasma spraying (VPS), as an alternative to bulk alloy manufacture. Drawing on our knowledge of "conventional" ODS bulk alloys, we will first learn how to make dense VPS coatings from powder. Then, any differences in microstructure and performance (e.g. microhardness) between coating and bulk will be investigated. Finally, particular focus will be given to understanding any differences in the development of the critical oxide dispersion.
Additive manufacture of heterogeneous composites for microwave communication applications

Patrick Grant

While much of the current focus on additive manufacture has concerned production of net shape 3D parts made from engineering polymers and alloys, arguably additive manufacture and 3D printing offers much greater impact for functional materials, where the function of interest is controlled point to point in 3D space according to a design requirement. Our group has been at the forefront of printing composites to produce graded and/or anisotropic composites that allow for novel manipulations of microwaves, through spatial variations in the composite permittivity and/or permeability. For example, we have recently 3D printed a compact microwave lens operating at 15 GHz (dx.doi.org/10.1002/admt.201600072). This project will explore the manufacture and characterisation of further implementations of our capability based on the idea of “filled voxels” in which 3DP is used to create a 3D array of empty voxels that are then filled, each with a material that may be either identical, or slightly or radically different from its neighbour according to a computer simulation-based design. The objective is to create novel 2D and 3D device morphologies for beam splitting, lensing, directional antenna, etc.

Superconducting solders for commercial MRI magnets

Chris Grovenor, Susie Speller

All MRI superconducting magnets contain superconducting joints that allow them to operate in persistent mode without any power consumption. At present these are made with a PbBi superconducting solder, but there are worries about future EU Pb-free directives and the optimum composition of the current solder. This project will, in collaboration with Siemens Magnet Technology, explore the microstructure and properties of new Pb-free solders and modifications to the existing materials and processes.

'Perfect' persistent mode joints for NbTi superconducting wire

Chris Grovenor, Susie Speller

All superconducting MRI magnets contain joints that allow them to operate in persistent mode, and these are made with a PbBi superconducting solder with properties much worse than the NbTi wires that they join.
This project will be a collaboration with Siemens Magnet Technology to explore a powder metallurgy approach to fabricate true NbTi to NbTi persistent joints. The student will make prototype joints, and will characterise them with analytical SEM and XRD techniques as well as measuring their superconducting properties.

**Joints for commercial high temperature superconducting tapes**

Chris Grovenor, Susie Speller

Large superconducting machines require long lengths of superconductor, but even after 20 years of development the best high field HTS tapes can only be produced in kilometer lengths. Thus many joints must be made in a large machine, and currently there is no successful process to do this. This project will explore the joining of commercial RE(BCCO) tapes [see Devices Course] using novel HTS solder concepts, and the student will correlate processing parameters with microstructure and superconducting properties.

**Characterisation and development of catalyst coatings for aerospace graded gas sensors**

Colin Johnston, Vitor Marques (Honeywell Aerospace)

Recently, there is an increased desire to monitor cockpit and cabin air quality during air transportation. For aerospace applications these sensors need to maintain performance during long periods of time while being resistant to cross contamination, such as fumes from the engine and anti-icing system. However, gas sensors resistance to contamination can be improved with the use of nano-catalyst coatings. This project aims to characterise and develop nano-catalyst coatings tailored to be compatible with aerospace environments. Existing coatings will be characterised in terms of microstructure, chemistry and surface properties (e.g. adhesion) and compared with newly developed coatings. Finally, their cross contamination performance will be accessed.

This project will be in collaboration with Dr Vitor Marques of Honeywell Aerospace and there will be some opportunity to visit them although the work will be primarily based at Begbroke.
In situ 3D observation of damage development and healing in a carbon-fibre/epoxy composite

James Marrow

The next generation of aerospace composites may have self-healing properties. A novel method for toughening and healing de-lamination damage in polymer composites, based on inkjet printing, will be investigated in collaboration with partners at Sheffield University.

You will use a high resolution X-Ray tomography microscope and will conduct experiments to observe de-lamination damage, in situ and in 3D, during mechanical tests of a carbon fibre-epoxy composite. Digital volume correlation measurement of the displacement field will quantify the microstructure deformation in an investigation of the criteria for damage propagation. You will design experiments to investigate the healing process, with the aim of understanding its contribution to the fracture resistance and to help optimise the composite design. There are opportunities for finite element modelling, if you are interested in this aspect, although this is not essential for a successful project.

The Toughness of Advanced Graphites for Generation IV Nuclear Fission

James Marrow

The next generation of high temperature nuclear fission reactors required advanced graphites with improved resistance to fast neutron irradiation damage. The irradiation changes the graphite's mechanical properties, and this has an impact on safe and economic operation. To optimise the advanced graphites being developed by our collaborators in China, we need new methods to quantify the fracture toughness of miniature test specimens that are currently being irradiated in a materials test reactor in the USA.

This project combines experiment design with modelling. You will study, in 3D with high resolution X-Ray tomography, cracks propagating within diametral compression test specimens of different candidate non-irradiated graphites. You will analyse these images by digital volume correlation to measure the 3D displacement field around the crack tip. These data provide the boundary conditions to calculate the toughness (i.e. critical strain energy release rate) via a finite element modelling analysis. The toughness will then be related to the graphite’s microstructure to help optimise the manufacturing process.
In Situ Characterisation of Strain Concentrations at Slip Bands and Twins
Interactions under applied loading

James Marrow

The intense localised deformation of twins and slip bands can be sufficient to initiate fracture, particularly in anisotropic metals such as zirconium, uranium and magnesium. Microstructure-informed design of alloys with improved mechanical performance requires data on the intensity of these interactions. It is now possible to quantify these via finite-element based methods, applied to full-field analysis of HR-EBSD data (High-resolution Electron BackScatter Diffraction); the measured strains are used to calculate the strain energy field.

This analysis method is under development, so the objective of this project is to examine the strain fields at blocked slip bands, twins and initiated cleavage cracks in a model material (age-hardened duplex stainless steel). This material has been chosen due to its suitability for EBSD (ease of sample preparation) and well characterised slip/twinning behaviour that is caused by 475°C embrittlement. You will design experiments for an in situ straining stage, using first optical and then scanning electron microscopy, leading to critical experiments to obtain HR-EBSD data. An interest in finite element modelling analysis is desirable, though not essential.

Nano-engineered stainless steel for advanced nuclear applications

James Marrow, Dong Liu

Nano-engineered stainless steels have been proposed to have superior resistance to irradiation-induced swelling, which is a limiting factor for fuel cladding for current and next generation reactors. This novel material, designed by Hong Kong City University, is expected to be irradiation tolerant. The first tests will be done with ion-irradiation to simulate the lifetime fast neutron dose. We need to know the effects of irradiation on yield and work hardening, but the shallow depth of ion damage can only be examined by micro mechanical testing (e.g. indentation).

You will work with un-irradiated material, exploring the correlation between the nanoscale microstructure and its mechanical properties. You will use nano-indentation to measure the hardness and elastic modulus, and examine the effects of heat-treatment up to 800°C.
We aim to apply a novel multiple sharp tip approach (in collaboration with Austrian Academy of Sciences) to derive the stress-strain behaviour by micro mechanical testing, for comparison with measurements you will make on the bulk material. This will support future work with ion-irradiated samples.

3D observation of damage evolution in synthetic diamond  
James Marrow, Dong Liu

Synthetic diamond has applications as diverse as the electronic, health care and oil industry, and is often employed as a composite or bonded material in which the properties of the interfaces are critical. You will examine a polycrystalline diamond, integrated with GaN for high power electronic devices that require excellent toughness for thermal shock resistance, and a sintered diamond with micro-meter grain size for wear resistance. The aim is to investigate the interfacial properties that control damage development.

You will use a high resolution X-Ray tomography to observe damage development, in situ and in 3D, during mechanical tests, analysed by digital volume correlation to quantify the displacement field and hence the distribution of damage. You will also measure residual stress using non-destructive techniques such as Raman spectroscopy. There will be an opportunity to integrate these measurements with finite element modelling to simulate damage development and to test the model against observation, although this is not essential for a successful project.

The effect of thermal aging on the atomic-scale microstructure and properties of 17-4PH steel  
Michael Moody, Maria Auger

17-4PH is a precipitation hardened martensitic steel widely used in the fabrication of structural components in power plants, aerospace or nuclear reactor applications due to its combination of good mechanical properties, wear resistance, and adequate corrosion resistance. The in-service conditions at high temperatures for very long times can induce long term embrittlement in the material, hence a better understanding of its aging response is critical in order to prevent failure. In the present project, in collaboration with Rolls Royce PLC, a 17-4PH steel will be subject to aging treatments at 350oC and 400oC for times up to 10000 h.
The evolution of the atomic-scale microstructure and mechanical properties at different aging times will be investigated by Atom Probe Tomography (APT) and complementary Vickers hardness measurements.

Enabling 3D Atomic-Scale Imaging of Hydrogen in Materials via Advanced Atom Probe

Michael Moody, Daniel Haley

The Atom Probe Research Group is undertaking leading research into the atomistic origins of Hydrogen Embrittlement (HE). HE is a critical issue and is highly prevalent across a diverse range of industries. To-date, we have undertaken HE research with our industrial partner, Rolls Royce PLC, who has strong interest in the development of hydrogen resistant alloys. These range from zirconium alloys and stainless steels for fission reactors to high strength steels for automotive and aerospace applications. This interest is sharpened as there does not exist any other technique which can identify the 3D distribution of hydrogen at the atomic scale, placing Atom Probe Tomography (APT) in a unique position.

Our research is underpinned by the development of new isotopic doping techniques combined with APT. We have developed novel instrumentation and methodologies for studying the interaction between gases and atomically clean surfaces, as well as the examination of samples electrolytically charged in heavy water. This project will continue the development of these techniques and in particular identify hydrogen trapping behaviour in HE relevant microstructures.

High-throughput interpretation of ensemble nanoparticle electron diffraction data

Peter Nellist, Lewys Jones

Electron diffraction patterns contain information about the atomic spacing of atoms and chemical ordering. Illuminating a selected area of the sample leads to a collective pattern covering many nanoparticles of differing orientations. These multiple-particle selected area electron diffraction (SAED) patterns allow for high-throughput measurements of ensemble sample properties.
The aim of this project is to evaluate the potential for using SAED for high-throughput analysis of nanoparticle systems as a function of particle size, composition, or exposure to heat, cold or gas environments. The aims are to measure crystal structure, strain and ordering in the case of alloys. If successful, this would enable real-time monitoring of in-situ nano-particle characterisation such as for accelerated ageing studies. Such measurements are crucial to enable rational design of future catalysts for energy applications.

This project can be tailored to the interest of the student to incorporate; hands-on experimentation including sample preparation and recording of electron diffraction patterns using the JEOL300F TEM, developing automated image-analysis techniques with computer programming in MatLab, or diffraction pattern simulation using GPU-based simulation codes.

**Increasing the recyclability of 6xxx series Al alloys for extrusions tbc**

Keyna O’Reilly, Marina Galano

About 90% of all Al alloys used for extrusions are 6xxx series Al-Mg-Si alloys. These alloys have good extrudability and formability together with superior mechanical properties and surface qualities. Extrusion billets are usually direct chill cast and homogenised before extrusion. There is on-going pressure to use more recycled materials in the casting industries, as this significantly reduces energy consumption and CO$_2$ emissions. However, recycled materials generally have a higher impurity content which leads to the formation of more, and possibly different, secondary phases forming in the alloys. There is on-going effort in developing advanced solidification technologies and extrusion processing technologies to tolerate higher impurity levels in extrusion billets. The influence of different cast microstructures on the extrudability is yet to be understood. In-addition, the as-cast secondary intermetallic phase inter-connectivity and the intermetallic type play critical roles in determining the extrudability of an alloy.

This project will aim to explore the microstructural evolution during extrusion of billets having different as-cast microstructures. An attempt will be made to correlate the final microstructure with extrudability, surface quality and mechanical properties of the alloys. DSC, XRD, OM, SEM and EDS will be used to characterise the materials. The outcome of this project will highlight how the initial as-cast microstructure can play a significant role in the extrudability of recycled materials.
Measuring inclusions in molten aluminium

Keyna O’Reilly

One key attribute of molten aluminium quality is the level of non-metallic inclusions present. Even though the concentration of inclusions is typically <1ppm, many products are very sensitive to these contaminants. The low concentration makes it difficult to quantify the inclusion content. The PoDFA (Porous Disk Filtration Apparatus) test developed in the 1960s is still widely used. A volume of melt is pressurised and passed through a very fine filter. Although a PoDFA tests 1.4kg of metal, the amount of metal effectively being “seen” by the metallographic technique is still only ~5g.

PoDFA measurements are characterised by large error bars, which increase relatively as the metal gets cleaner. Very dirty metal with a PoDFA level ~1.0mm²/kg might have a measurement error +/-10%. In contrast, cleaner metal with a level of 0.01-0.001mm²/kg would exhibit a measurement error of +/-100% or more. Given the time required for a single analysis (~2hours), very few PoDFA users undertake repeat measurements, and thus often do not appreciate the errors involved.

Inclusion analysis

The standard PoDFA technique still entails metallographically examining many fields of view in a microscope, and estimating the area fractions of inclusions. It would be interesting to apply a range of modern analytical techniques to analyse inclusions present on a PoDFA filter. These could include for example:

- SEM automated image analysis of standard PoDFA sample
- Taper sectioning of the filter, with SEM automated image analysis
- Butanol dissolution of the filtrate, followed by XRD analysis
- 3-D X-ray tomographic analysis of inclusion distribution on filter (using low Fe alloy)

The objective is to develop a more accurate analysis of the inclusion content in liquid metal. At the very least this would be applicable to scientific studies, but could well have application as a production quality tool.

This work is a joint collaboration with our technical partners TSC.
About 90% of all Al alloys used for extrusions are 6xxx series Al-Mg-Si alloys, and the vast majority of these materials will have been cast by Direct Chill (DC) casting. Non-equilibrium solidification in DC casting results in the formation of highly interconnected secondary phases during the final stages of solidification. In dilute extrudable 6xxx series Al alloys these phases are $\alpha$-AlFeSi and $\beta$-AlFeSi intermetallics which have different compositions, crystal structures and properties. Their presence in DC cast billet significantly affects its extrudability. Homogenisation can improve extrudability by eliminating the as-cast micro-segregation and breaking-up the intermetallic's interconnectivity by promoting a phase transformation of $\beta$ to $\alpha$. This phase transformation is still not clearly understood. 

This project will aim to optimise the homogenisation practice by (a) understanding the microstructural evolution during homogenisation of DC cast billets having different as-cast microstructures, and (b) exploring the mechanism of $\beta$-AlFeSi to $\alpha$-AlFeSi transformation. A hot stage attached to an optical microscope will be used to observe the real time phase transformation. DSC, XRD, SEM and EDS will be used to characterise the materials. The potential outcome of this work will be to understand how the initial as-cast microstructure plays a role in the intermetallic phase selection during homogenisation and whether it is feasible to eliminate the homogenisation practice completely by controlling the formation of a favourable microstructure during casting.

**DC casting simulator – does it work for intermetallic phases?**

The vast majority of wrought Al alloy billets and ingots are direct chill (DC) cast. Before each cast, industry will carry out what is termed a “TP-1” test, which samples a small volume of metal and solidifies it in a reproducible way. This sample is then sectioned in a prescribed way and the grain size is measured. There is good evidence to believe that the grain size obtained will be representative of the grain size in the DC cast billets (with potentially many tonned of metal being cast at a time). The DC cast microstructure comprises an Al matrix and a number of secondary intermetallic phases. We have analysed the intermetallics in a TP-1 test and compared them to those in a DC cast billet.
Whilst the TP-1 sample produces the correct types and proportions of the intermetallics present, it does not produce exactly the same morphologies and distribution of the intermetallics. We have had built an alternative DC casting simulator, and we would like to investigate whether this is a better simulator of the intermetallics present in DC casting.

This project will use an extraction technique to dissolve away the Al matrix and reveal the 3D interconnected structure of the intermetallics. These can then be compared with intermetallics from DC cast billets. DSC, XRD, OM, SEM and EDS will be used to further characterise the materials. The hope is that this project will demonstrate that the DC casting simulator can accurately predict, using a relatively small quantity of molten metal, the intermetallic types, proportions, morphologies and distributions, so enabling small scale experiments to replace full scale DC casts.

**Metal anodes in Ionic Liquids**

Mauro Pasta

The lithium-ion batteries that power our laptops, smartphones and electric vehicles could have significantly higher energy density if their graphite anodes were to be replaced by lithium metal anodes. Obstructing this change, however, has been the formation of dendrites, microscopic fibers of lithium that sprout from the surface of the lithium electrode and spread across the electrolyte until they reach the other electrode thus short-circuiting the battery. Ionic liquids (ILs) represent a very interesting new class of room temperature fluids. The main advantages of ILs towards organic solvents are non-flammability, negligible vapor pressure, high chemical and thermal stability. In this project the student will investigate the effect of different ionic liquids on the electrochemistry and dendrite formation problem on Li and Na metal anodes.

**Cathode materials for Mg-ion batteries**

Mauro Pasta

Magnesium metal is an ideal rechargeable battery anode material because of its high volumetric energy density, high negative reduction potential and natural abundance. Coupling magnesium with high-capacity, low-cost cathode materials would lead to a new generation of batteries able to satisfy the always-increasing energy demands of the new generation of portable devices and electric vehicles.
In this project the student will work on characterizing how open-framework crystal structure materials could potentially represent the ideal cathode material candidate for secondary Mg-ion batteries applications.

**Mixed-Metal Fullerene Molecular Magnets**

Kyriakos Porfyrakis

Incorporation of strongly paramagnetic ions inside fullerene cages like Dy, Sc and Gd can lead to the formation of fullerene Single Molecule Magnets that can find applications in Quantum Information Processing, spintronics and in nanomedicine as Magnetic Resonance Imaging contrast agents. The project involves the synthesis of mixed metal endohedral metalofullerenes through an arc discharge vaporization procedure and the study of their electronic transport and magnetic properties.

**Endohedral Fullerene - Plasmonic Nanoparticles Dyads**

Kyriakos Porfyrakis

The project involves the synthesis of dyads between endohedral fullerenes and plasmonic nanoparticles such as gold in order to enhance the fullerene photoluminescence properties. The coupling between the fullerene and the nanoparticle will be modulated via controlling the length of the bridge molecule. The photoluminescence of the dyad structure will be assessed by PL spectroscopy. Any enhancement of the PL intensity is expected to lead to more efficient optical fibres, sensors and fluorescent labels.

**Synthesis of N@C60 for Molecular Atomic Clocks**

Kyriakos Porfyrakis, Edward Laird

N@C60 has recently been hailed as the world's most valuable material! A pocket size atomic clock would have the potential to revolutionise communication and navigation. We have a unique approach based on endohedral fullerenes. We have the most advanced factory for N@C60 synthesis but the yields are still far lower than required. The project involves process optimization for the synthesis of N@C60 via ion implantation. Process parameters will be modified in order to improve the yield of N@C60. The student will also be expected to contribute towards low frequency EPR (electron paramagnetic resonance) experiments, measuring atomic clock transitions.
Nanofabrication of graphene and TDMCs using ion beam milling

Jason Smith, Aurelien Trichet

This project will explore the ability to fabricate nanostructured devices in graphene and in 2-dimensional transition metal dichalcogenide (TMDC) semiconductors using focused ion beam (FIB) milling. FIB is a highly controlled technique for nanofabrication with spatial resolution of under 10 nm. Here you will use the instrument to produce nanoscale holes in 2D materials, image them in an electron microscope and measure their optical properties using optical microscopy and spectroscopic techniques. The aim will be to measure localised plasmons and polaritons (free electron oscillations and hybrid particles of photons and excitons) that can be used for quantum light sources and nanoscale biosensor devices.

Photonic structures for quantum light sources in diamond

Jason Smith, Sam Johnson

This project will involve the fabrication and testing of photonic structures in high purity diamond to evaluate their use in controlling optical emission from single point defects. The structures will be produced by focused ion beam milling of synthetic diamond. This will be done around existing point defects and the effect on photon emission measured using optical microscopy and spectroscopy and photon correlation techniques. The aim will be to produce structures that generate directional emission from single nitrogen-vacancy defects for high efficiency single photon source devices. You will receive training in all aspects of fabrication and characterisation from members of the Photonic Nanomaterials Group.

Nanodiamond single photon sources

Jason Smith

Single point defects in nanodiamond offer great potential as single photon sources in quantum technologies, and many laboratory demonstrations have been carried out to show their basic properties. However robustness of the single photon emission properties is a persistent issue - after a period of time the emission can become unstable or switch off altogether as a result of changing surface charge and chemistry of the nanodiamonds.
The goal of this project is to identify nanodiamond materials and simple processing methods that offer robust single photon emission properties. Materials will be sourced from a variety of suppliers, and your task will be to characterise their optical properties, identify the most promising samples, try out processing steps such as annealing, acid cleaning, and etching, and recharacterise to measure improvements in the properties. Your results will feed into an existing program to build a prototype single photon source device with industrial partner ID Quantique.

**Ultraclean carbon nanotubes for novel superconducting quantum devices**  
Susie Speller, Edward Laird

Carbon nanotubes are the smallest semiconducting wires that exist. In ‘ultraclean’ fabrication, nanotubes are grown chemically and assembled into devices in a way that preserves their pristine atomic structure. This has made possible new kinds of qubits and nanoscale mechanical resonators. This project will make novel quantum devices using the combination of nanomaterials and superconducting electronics, using state-of-the-art deposition facilities. You will explore two kinds of superconducting contact material: MoRe alloys that survive the harsh conditions used in nanotube growth; and Nb alloys onto which clean nanotubes can be transferred. The aim will be to optimize the superconducting critical current, and eventually to use these nanotube junctions in new devices to study quantized vibrations in nanoscale devices.

**Superconducting thin films for highly efficient quantum resonators**  
Susie Speller, Chris Grovenor

Quantum devices based on single electronic charges need to be connected by highly efficient, low power circuits. One way of building these circuits is with superconducting resonator structures, and (Ti,Nb)N is an effective material for this purpose. This project, in collaboration with quantum device researchers in the department, involves the deposition of high quality nitride thin films. A wide range of techniques will be used to characterise the microstructure and superconducting properties of the films to optimise performance in quantum circuits.
Persistent mode joints between high temperature superconducting wires

Susie Speller, Chris Grovenor

All large superconducting magnets contain superconducting joints that allow them to operate in persistent mode without any power consumption. This project is a collaboration with a magnet manufacturer, Oxford Instruments, to investigate ways to make persistent mode joints between high temperature superconducting Bi2Sr2CaCu2O8 wires. The student will make prototype joints by developing a local melting process, and will characterise them with analytical SEM and XRD techniques as well as measuring their superconducting properties.

Magnesium diboride bulk materials for medical applications

Susie Speller, Chris Grovenor

Magnetic Resonance Imaging (MRI) is a very widely used technique for medical diagnosis, but the current instruments based on superconducting solenoids are large and expensive. There are emerging designs for smaller and cheaper instruments based on bulk superconductors such as MgB2 acting as permanent magnets. This project involves collaborating with industrial partner Element6 in the fabrication of bulk MgB2 superconductor by hot pressing. The student will correlate processing parameters with microstructure and superconducting properties, aiming to optimise the trapped field.

Discrete dislocation modelling of uranium

Edmund Tarleton, James Marrow

α-uranium is an orthorombic crystal with plastic slip dominated by edge dislocations on the (010)[100] and {110}<1-10> slip systems. The fracture of uranium is sensitive to the different strain behaviour of adjacent grains, and there is work in progress to develop polygranular 'crystal plasticity' models. The plastic deformation in a single crystal can conveniently be simulated in 2D. This is fundamental to the polygranular models. An isotropic 2D discrete dislocation plasticity code has been developed in Matlab, and will be applied to uranium in this project. You will first learn the principles of dislocation modelling, calibrate the input parameters for uranium and then perform some large scale simulations of compression and tension. The model may then be extended to include either elastic anisotropy or fracture.
Predicting the role of grain structure during the deformation of metallic polycrystals

Edmund Tarleton, David Collins

A combination of experiments and modelling will be used to study how dislocations interact and accumulate in the vicinity of grain boundaries for automotive high strength steels. A currently available computational tool called crystal plasticity finite element modelling will be developed to incorporate grain morphology and local orientation, to enable the study of localised deformation due to the character of grain structure. The models will be validated with high resolution electron backscatter diffraction (HR-EBSD), providing measurements of grain structures and a quantification of the dislocation content.

Dislocation modelling of micro seesaw experiments

Edmund Tarleton, Angus Wilkinson

The Bauschinger effect is normally associated with a decrease in the flow strength of a metal when the direction of strain is changed. The mechanism is related to the dislocation structure in the cold worked metal. During deformation, dislocations accumulate at barriers and produce dislocation pile-ups and tangles. Discrete dislocation simulations will be performed with a user friendly matlab code being developed by the group in Oxford. The aim will be to simulate and understand state of the art micro-scale 'seesaw' tests on single crystals currently being performed in the micromechanics group. The student will be working closely with the supervisors and with experimental researchers in Oxford.

Flash sintering of ceramics

Richard Todd

Normally, it takes several hours at a temperature in excess of 1000 C to sinter a ceramic. However, it has recently been discovered that this can be achieved in a few seconds with furnace temperatures below 1000 C by applying a voltage to the specimen whilst it is heated. We have successfully repeated the result and have established that the "flash event" originates in a thermal runaway effect. The project aims to investigate and exploit the rapid sintering and deformation which accompanies the power surge of the flash event.
Cyclic fatigue of Y-TZP ceramics

Richard Todd

Zirconia is used for hip joint replacements and dental implants because of its high toughness. These applications involve cyclic loading and are therefore potentially susceptible to fatigue failure. Recent work in Oxford has shown that this is indeed an issue in Ce-TZP, possibly due to reversibility of the t to m transformation. The project will extend the investigation and apply it to the more common Y-TZP composition. The work will involve mechanical testing and Raman microspectroscopy to map the phase content around the cracks.

"Cold sintering" of ceramics

Richard Todd

Very recently, it has been reported that "reactive liquid phase sintering" of ceramics can be achieved by using water based solutions as the liquid phase rather than a high melting point glass. This reduces the sintering temperature from >1000 C to close to room temperature. The project aims to reproduce this astounding result, to investigate it further and to develop it as an energy saving processing method for ceramics.

Indentation Damage in Advanced Ceramics

Richard Todd, James Marrow

Indentation of ceramics is a complicated process which forms the basis of several standard tests and is also relevant to practical applications. However, the details are still not well understood, partly because it is difficult to study the processes that occur under the indentation. This project will use X-ray computed tomography (XCT), which can be applied with sub-micron resolution to materials that are opaque to visible light to investigate the damage occurring during indentation, conducted in situ. The 3D datasets obtained will be analysed by digital volume correlation methods (DVC) to measure the full field displacements that arise from damage and cracking.
Quantum Dot Photovoltaics

Andrew Watt

The efficiency of solution processed lead chalcogenide colloidal quantum dot (CQD) solar cells has increased from less than 1 to over 11% in the last 8 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 Synthesisis 2. CQD Device Characterisation 3.CQD TEM. All projects will involve the fabrication of devices.

Cold Dwell Effects in Ti Alloys

Angus Wilkinson, David Collins, David Armstrong

In room temperature fatigue of Ti alloys holds at peak loads can have a profound effect reducing the fatigue life by a factor of 10. This is thought to be linked to small amounts of time dependent plastic deformation - creep under fixed load, or stress relaxation under fixed strain. This project will explore effects of oxygen content on cold dwell response of commercially pure Ti. Digital image correlation and high resolution EBSD will be used to characterise local distributions of plastic and residual elastic strains at the grain level and how they relate to the microstructure.

Macrozones in Ti Alloys - Rapid Orientation Mapping using Polarised Light

Angus Wilkinson, Jicheng Gong, David Collins

Alpha-Ti alloys often contain macrozones which are large multi-grained regions with similar crystal orientation inherited from large prior beta-grains present in earlier processing steps. These macrozones can have profound effects on the alloy performance but may go un-noticed in conventional optical or SEM imaging. This project will develop methods of mapping c-axis orientations using multiple polarised light microscope images. The method will allow rapid mapping of large areas and could be combined with serial sectioning for 3D mapping of these technologically important macrozone structures.
Effect of Grain Boundaries on Short Fatigue Crack Growth

Angus Wilkinson, Jicheng Gong

Fatigue is a pervasive failure mode that remains a source of in-service failure on the one hand and inefficient conservative design on the other. We have developed a novel ultrasonic (20 kHz) testing methodology capable of applying a high number of cycles in a short timeframe to small sample volumes spanning a few 100 microns. The rig will be used to measure the retardation and acceleration of microstructurally short cracks as they interact with grain boundaries. Automated in situ optical microscopy will be complemented with intermitent SEM, EBSD and AFM measurements to give mechanistic insight.

Defect engineering for multicrystalline silicon solar cells.

Peter Wilshaw, Phillip Hamer

This project will study methods by which the electrical effects of the harmful impurities in the silicon solar cells can be reduced and thus its ultimate aim is to reduce the cost and/or improve the efficiency of practical solar cells. The research will involve some processing of solar cell material in the Begbroke clean room and characterisation techniques such as quasi-steady state photoconductance decay (QSS-PCD). Some basic electrical characterisation such as IV and CV measurements will also be included.

Novel Photon Capture Methods for Silicon Solar Cells

Peter Wilshaw, Phillip Hamer

This project concerns improving the performance of crystalline silicon solar cells, which account for over 90% of all currently manufactured solar cells. Texturing of multicrystalline silicon wafers for solar cell production has been an ongoing concern for cell manufacturers. The student will evaluate novel texturing approaches for multicrystalline silicon involving liquid and gas-phase etching. Post processing will be performed in the Begbroke clean room and the material will be characterised using a variety of optical and electricval methods.
Surface Passivation For Silicon Solar Cells

Peter Wilshaw, Sebastian Bonilla

The surfaces of solar cells act as defects and thus promote electron hole recombination that reduces the efficiency of the cells. The semiconductor group at Oxford has developed processes to produce record reductions in carrier recombination at surfaces (passivation). This project will require the student to continue this work looking at how the processes may be optimised and performing accelerated aging measurements to assess their stability. Work will take place both on the main site and in the Begbroke clean room.