# DEPARTMENT OF MATERIALS

# PART II PROJECTS

# 2019/2020

**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 5th February 2019 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 2019.

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:

| Name | Room | Building | Tel. No. |
|---|---|---|---|
| Dr Natalia Ares | 20.09 | 12/13 Parks Rd | 73719 |
| Prof David Armstrong | 20.08 | 21 Banbury Road | 73708 |
| Prof. Hazel Assender | 30.06 | Hume-Rothery Building | 73781 |
| *(On 5th February, Prof Assender only available from 2.30-3pm, then 4.30pm onwards; and will be in her office on the morning of Thursday 7th February* ***apart from 10-11am****)* | | | |
| Prof. Harish Bhaskaran | 40.21 | Engineering & Technology Bldg | 73772 |
| *(Prof Bhaskaran is in his office on 5th February 2.30-3pm. Please email: harish.bhaskaran@materials.ox.ac.uk for an appointment to discuss his projects)* | | | |
| *Prof Andrew Briggs* | *30.05* | *12/13 PR* | *73725* |
| *(Prof Briggs is not available on 5th February, please see Natalia Ares)* | | | |
| Dr Lapo Bogani | 195.40.03 | 16 Parks Rd | 83341 |
| Prof. Peter Bruce ~4pm | 10.09 | Rex Richards Building | 12761 |
| *(Upon arrival at Rex Richards Building please dial "energy" and you will be met by Zsofia Lazar, Peter Bruce's PA. Room 10.09 is on the* ***ground floor*** *of the Rex Richards building. Note:* ***Peter Bruce*** *will not be in Oxford on 5th February, but senior members of his team will be available to discuss the projects proposed).* | | | |
| Prof Jan Czernuszka | 10.15 | 21 Banbury Rd | 73771 |
| Prof Nicole Grobert | 317.20.09 | Begbroke Science Park | 83720 |
| *(Please email Prof Grobert nicole.grobert@materials.ox.ac.uk for an appointment at Begbroke)* | | | |
| *Prof Chris Grovenor* | *50.12* | *Engineering & Technology Bldg* | *73751* |
| *(Prof Grovenor is not available on 5th February. Prof Grovenor and *Prof Speller will hold a session in the Holder café on* ***8th February*** *from 2pm onwards)* | | | |
| Prof. James Marrow | 10.18 | 21 Banbury Road | 73938 |
| Prof. Peter Nellist | 30.05 | Holder Tower | 73656 |
| Rebecca Nicholls | tbc on 5th February | | |
| Prof Sergio Lozano-Perez | 30.06 | Holder Tower | 73795 |
| Prof M Pasta | 40.29 | Rex Richards (lab) ask for Mauro: | 12991 |
| *Prof Roger Reed* | | *Rex Richards* | *13069* |
| *(Prof Reed location on 5th February tbc)* | | | |
| Prof Jason Smith | 195.30.10 | 12/13 Parks Road | 73780 |
| *(Prof Smith only available until 5pm on 5th February)* | | | |
| Prof. Susie Speller | 20.05 | 21 Banbury Road | 73734 |
| *(Prof Speller will be in the Holder café until 4pm on 5th February. *Prof Speller and Prof Grovenor will hold a joint session in the Holder café on* ***8th February*** *from 2pm onwards)* | | | |
| Prof. Richard Todd | 40.20 | Engineering & Technology Bldg | 73718 |
| Prof Jamie Warner | 195.20.03 | 12/13 Parks road | 73790 |
| Prof. Angus Wilkinson | 10.19 | 21 Banbury Road | 73792 |

| | | | |
|---|---|---|---|
| *Prof. Peter Wilshaw* | *50.15* | *Engineering & Technology Bldg* | *73736* |

*(Prof Wilshaw will not be in Oxford until 11th February, please email peter.wilshaw@materials.ox.ac.uk to make an appointment to discuss the projects)*

| | | | |
|---|---|---|---|
| Prof Jonathan Yates | | 15 Parks Rd | 12797 |
| Prof Neil Young | 30.13 | Holder Building | 73655 |

## PROJECTS ON OFFER:

**Micromechanical investigation of interfacial properties of SiC-SiC fiber composites for nuclear applications by push-out method ..... 8**
David Armstrong Co-Supervisor(s): Yevhen (Eugene) Zayachuk ..... 8

**Macro-Mechanical Testing of Novel High-Entropy Alloys for Nuclear Application ..... 8**
David Armstrong Co-Supervisor(s): Angus Wilkinson, Dr Bo Shiuan-Li ..... 8

**Effect of Irradiation Damage on Plastic Zone Morphology around nanoindentations in Zirconium ..... 9**
David Armstrong Co-Supervisor(s): Anna Kareer, Phani Karamched, Angus Wilkinson ..... 9

**Mechanical properties of solid state lithium ion batteries ..... 9**
David Armstrong Co-Supervisor(s): Ed Darnborough ..... 9

**Phase separation and properties of polymer dispersed liquid crystals ..... 10**
Hazel Assender ..... 10

**Characterization of gas-barrier polymer films ..... 10**
Hazel Assender ..... 10

**Evaporated molecular semiconductors for flexible electronics ..... 11**
Hazel Assender ..... 11

**Active photonic materials for next-generation computing ..... 11**
Harish Bhaskaran ..... 11

**Fabrication and testing of nanoscale devices using new materials ..... 11**
Harish Bhaskaran ..... 11

**Ab-initio energy considerations on molecular graphene defects ..... 12**
Lapo Bogani Co-Supervisor(s): Colin Lambert (Lancaster Uni) ..... 12

**Light-induced relaxation dynamics in the Brown-Neél model ..... 12**
Lapo Bogani ..... 12

**Analysis of multi-centre spin anisotropy using torque magnetometry ..... 12**
Lapo Bogani ..... 12

**Analysis of multi-centre spin anisotropy using torque magnetometry ..... 12**
Lapo Bogani ..... 12

**Analysis of multi-centre spin anisotropy using torque magnetometry ..... 13**
Lapo Bogani ..... 13

**Thin-film resonators for quantum devices ..... 13**
Andrew Briggs Co-Supervisor(s): Natalia Ares, Susannah Speller ..... 13

**Automated readout of semiconductor qubits ..... 13**
Andrew Briggs Co-Supervisor: Natalia Ares ..... 13

**Cavities for sensitive read-out of mechanical motion ..... 14**
Andrew Briggs Co-Supervisor: Natalia Ares ..... 14

**Oxygen redox chemistry in Li-ion and Na-ion battery electrode materials ..... 14**
Peter Bruce ..... 14

**Building the batteries of the future - solid-state synthesis and electrochemicaltesting of superionic conductors for all-solid-state battery applications ..... 14**
Peter Bruce ..... 14

**Fabrication of 3D printed gas diffusion electrodes for Li-air batteries ..... 15**
Peter Bruce ..... 15

**All natural composites ..... 15**
Jan Czernuszka ..... 15

**Dynamic Mechanical Analysis of Natural Tissues ..... 15**
Jan Czernuszka ..... 15

**Aerogel synthesis towards targeted applications ..... 15**

Nicole Grobert ........................................ 15

**Nanomaterials for Thermal Management in Electronics ........................................ 16**
Nicole Grobert ........................................ 16

**Synthesis and application of ternary transition metal fluoride nanoparticles on carbon support structures ........................................ 17**
Nicole Grobert ........................................ 17

**Designing and testing fibre laminate composites free of carbon fibres for thermal applications ........................................ 17**
Nicole Grobert Co-Supervisor(s): Roger Reed ........................................ 17

**Production and mechanical testing of hierarchical composite structures by freeze casting for energy, thermal, or structural applications ........................................ 18**
Nicole Grobert Co-Supervisor(s): Richard Todd ........................................ 18

**Joints in practical superconductors ........................................ 18**
Chris Grovenor Co-Supervisor(s): Susie Speller ........................................ 18

**The effect of nitrogen on the properties of thin film solid state electrolytes ........................................ 19**
Chris Grovenor Co-Supervisor(s): Susie Speller, Stefanie Zekoll ........................................ 19

**Spray casting solid state electrolyte thin films ........................................ 19**
Chris Grovenor Co-Supervisor(s): Susie Speller, Stefanie Zekoll ........................................ 19

**New Zr alloys for fusion applications ........................................ 19**
Chris Grovenor Co-Supervisor(s): David Armstrong ........................................ 19

**Scalable HRTEM image simulation of nanoparticles for machine learning dataset generation 20**
Professor A I Kirkland ........................................ 20

**Atomic resolution electric field mapping ........................................ 20**
Professor A I Kirkland ........................................ 20

**Understanding the role of oxide porosity in stress corrosion cracking ........................................ 22**
Sergio Lozano-Perez Co-Supervisor(s): Chris Grovenor ........................................ 22

**Cracks in heterogeneous materials, quantified in 3D by in situ X-ray tomography and Digital Volume Correlation ........................................ 22**
James Marrow Co-Supervisor(s):Yang Chen ........................................ 22

**In situ Studies of the Deformation of Highly Porous 3D CNT tube (CNTT) Networks. ........................................ 23**
James Marrow Co-Supervisor(s): Nicola Pugno (Trente University ........................................ 23

**Fracture of Novel Graphites for Next Generation Nuclear Energy ........................................ 23**
James Marrow ........................................ 23

**Cracks in heterogeneous materials, quantified in 3D by in situ X-ray tomography and Digital Volume Correlation ........................................ 24**
James Marrow Co-Supervisor(s):Yang Chen ........................................ 24

**Investigating nanoscale solute cluster formation mechanisms in high-strength aluminium alloys by atom probe tomography ........................................ 25**
Michael Moody Co-Supervisor(s): Paul Bagot ........................................ 25

**Mapping strain by electron diffraction and imaging ........................................ 25**
Pete Nellist ........................................ 25

**Understanding Screw Dislocation Structures in BCC metals ........................................ 25**
Pete Nellist Co-Supervisor(s): Dave Armstrong........................................ 25

**Modelling the imaging of bonding in materials by combining electron microscopy with density functional theory ........................................ 26**
Pete Nellist Co-Supervisor(s): Jonathan Yates, Rebecca Nicholls........................................ 26

**Batteries for grid-scale energy storage ........................................ 26**
Mauro Pasta ........................................ 26

**Laser written qubits in wide band gap crystals ........................................ 27**
Jason Smith ........................................ 27

**Measuring atmospheric aerosols with microcavity sensors ........................................ 27**

Jason Smith ........................................................ 27

**Triggered single photon sources based on point defects in solids ........ 28**
Jason Smith ........................................................ 28

**Microstructure of MgB2 bulk magnets ........................................ 28**
Susie Speller Co-Supervisor(s): Chris Grovenor ........................ 28

**Nacre-like alumina ceramics ................................................ 28**
Richard Todd Co-Supervisor(s): Nicole Grobert ......................... 28

**Synthesis of 2D materials by chemical vapour deposition .................. 29**
Jamie Warner ....................................................... 29

**Dislocation Loops in Irradiated Metals – effects on diffraction peak broadening ...... 29**
Angus J Wilkinson Co-Supervisor(s): Ed Tarleton ...................... 29

**Fatigue crack initiation in austenitic stainless steels .................. 30**
Angus J Wilkinson Co-Supervisor(s): Jicheng Gong ..................... 30

**Nano-scratch testing: Understanding fundamentals of wear ................ 30**
Angus J Wilkinson Co-Supervisor(s): Anna Kareer ....................... 30

**Novel Texturing Processes for Silicon Photovoltaics manufacturing ........ 31**
Peter Wilshaw Co-Supervisor(s): Sebastian Bonilla ..................... 31

**New surface passivation processes for silicon solar cells ................ 32**
Peter Wilshaw Co-Supervisor(s): Sebastian Bonilla ..................... 32

**Using DFT to interpret spectra from atomic vibrations in the electron microscope ...... 32**
Jonathan Yates Co-Supervisor(s): Rebecca Nicholls ..................... 32

**DFT modelling of the effect of carbon additions on grain boundary toughness in alumina ...... 33**
Jonathan Yates Co-Supervisor(s): Richard Todd ......................... 33

**Nanogalvanic reactions studied via TEM ..................................... 33**
Neil Young Co-Supervisor(s): Richard Compton (Chemistry) .............. 33

**Electron microscopy studies of electrochemical transformations .......... 33**
Neil Young Co-Supervisor(s): Richard Compton (Chemistry) .............. 33

**Micromechanical investigation of interfacial properties of SiC-SiC fiber composites for nuclear applications by push-out method**

**David Armstrong** Co-Supervisor(s): Yevhen (Eugene) Zayachuk

SiC SIC Composites are a leading candidate material for next generation nuclear power and aero engine applications. Our industrial partner – General Atomics – have provided us a set of miniaturized SiC-SiC composite samples, with different types of fibers and different types of interphases. We will use newly developed methods in our group to characterize the mechanical properties of these interfaces. The student will learn SEM and EDX and use them to characterize microstructure of these materials. He or she will also learn nanoindentation and push-out testing methods and develop a procedure for push-out of a miniaturized samples. Ultimately, hardness and modulus measured by nanoindentation will be correlated with microstructures of different fibers, and interfacial strength measured by push-out – with structures of different interphases.

**Macro-Mechanical Testing of Novel High-Entropy Alloys for Nuclear Application**

**David Armstrong** Co-Supervisor(s): Angus Wilkinson, Dr 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 (four-point bending, compression, up to 600 °C and digital image correlation) 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.

**Effect of Irradiation Damage on Plastic Zone Morphology around nanoindentations in Zirconium**

**David Armstrong** Co-Supervisor(s): Anna Kareer, Phani Karamched, Angus Wilkinson

Zirconium is a key material used in the fuel cladding in nuclear fission pressurized water reactors. During service it will be subjected to high levels of irradiation damage from neutrons. How these materials behave mechanically after irradiation is important for the design of future nuclear reactors, especially how the active slip systems in HCP zirconium can change.

Due to the difficultly 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 pure zirconium. 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. The student will gain experimental experience of SEM, AFM and diffraction techniques and develop analytical skills in matlab.

**Mechanical properties of solid state lithium ion batteries**

**David Armstrong** Co-Supervisor(s): Ed Darnborough

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.

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.

**Phase separation and properties of polymer dispersed liquid crystals**

**Hazel Assender**

Polymer dispersed liquid crystals are used to create optically switchable devices/panels and have also been of recent interest for microfluidic waveguide and haptic applications. They exploit the ability of the liquid crystal phase to reorientate to change the optical or mechanical properties, or shape, of the composite. Often the micro-scale composite structure is formed by a phase separation process on curing of a thermosetting matrix, and to date most studies have focussed on thermal curing. In this project a radiation curable system could be explored which would have the advantage of allowing of localised control of curing to make more complex structures. LC/PDMS composites will also be considered for their application in waveguides and the possibility of create dynamically controllable shapes/stiffness of material e.g. for soft and haptic contact in robotic or healthcare applications.

**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. Our recent development of the ‘Ca test method’ reveals the microstructure of WV permeation and allows quantification of the different permeation mechanisms that we seek to explore in novel layers. The project may give the opportunity to work in partnership with industry.

**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.

**Active photonic materials for next-generation computing**

**Harish Bhaskaran**

This project would look into how to choose active photonic materials for creating the next generation of computing devices that use light instead of electricity. It would involve both creatively choosing new materials as well as characterizing various materials to use on photonic devices. As a research project the student would learn how to use their knowledge and combine it with knowledge they would glean from various resources independently to help the research group achieve their aims and objectives.

**Fabrication and testing of nanoscale devices using new materials**

**Harish Bhaskaran**

This project would involve the Part II student learning how to make nanoscale devices in a device fabrication laboratory. They would learn valuable skills in fabrication and testing devices, This is a core experimental project that involves lots of interesting but time consuming work, with the added benefit of havng the satisfaction of making a device that may work well. As a research project the student would learn how to use their knowledge and combine it with knowledge they would glean from various resources independently to help the research group achieve their aims and objectives.

### Ab-initio energy considerations on molecular graphene defects

**Lapo Bogani** Co-Supervisor(s): Colin Lambert (Lancaster Uni)

This project will address the presence of diamagnetic and spin-bearing defects in the synthesis of polycyclic aromatic molecules. The project will consider the computational problems posed by the calculation of the energetic and entropic contributions in the formation of defects in synthetically-made graphene. The project will be carried out in the scope of an ongoing collaboration with the University of Lancaster (Prof. Colin Lambert).

### Light-induced relaxation dynamics in the Brown-Neél model

**Lapo Bogani**

The project will address, from a theoretical perspective, the relaxation mechanism of magnetic nanoparticles following the Brown-Neél superparamagnetic dynamics. The project will then consider the behaviour of ensembles of nanoparticles with a distribution of sizes, and will eventually study the effect that light can have on the magnetization dynamics of such systems, e.g. by inducing plasmonic resonances.

### Analysis of multi-centre spin anisotropy using torque magnetometry

**Lapo Bogani**

The project will study the role of the presence of several non-collinear spin centres on the magnetic torque effect. The project will produce the data-analysis tools necessary to determine the orientation of the centres from angle-resolved and magnetic-field swept torque measurements at cryogenic temperatures.

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### Thin-film resonators for quantum devices

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

Thin-film superconductors can be used to fabricate electromagnetic cavities, which trapping photons, 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 the displacement of nanomechanical resonators. Students that are keen on nanofabrication and the superconducting properties of materials will find this project particularly exciting.

### Automated readout of semiconductor qubits

**Andrew Briggs** Co-Supervisor: Natalia Ares

The development of quantum computers requires hundreds to millions of physical qubits to be read-out with high fidelity. Automatization of this process, which takes weeks of human effort, is essential for scalability. The focus of this project is to apply machine learning techniques to automatize the tuning of electrometers in semiconductor devices. The project involves a collaboration with machine learning experts. If you are passionate about quantum technologies and computer coding, this is a project for you!

**Cavities for sensitive read-out of mechanical motion**

**Andrew Briggs** Co-Supervisor: Natalia Ares

We are experimentally studying cavities that can trap radio-frequencies or microwaves to gain exquisite control of the vibrations of very thin membranes. The aim of this project is to optimize the interaction of 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 the mechanical properties of materials and light-matter interactions.

**Oxygen redox chemistry in Li-ion and Na-ion battery electrode materials**

**Peter Bruce**

Reversible reduction and oxidation of oxide ions in intercalation materials offers an interesting route to increase the energy density of next-generation Li-ion rechargeable batteries. This project will involve synthesis and characterisation of new Li-ion and Na-ion intercalation compounds which will be assembled into batteries and tested to examine their structural and electronic behaviour during operation with the aim of understanding O-redox chemistry in more depth. The student will gain a wide base of knowledge covering battery electrochemistry, solid state structural chemistry and various spectroscopic techniques.

**Building the batteries of the future - solid-state synthesis and electrochemicaltesting of superionic conductors for all-solid-state battery applications**

**Peter Bruce**

This project will build on the solid-state chemistry and electrochemistry taught in the Part I chemistry course. The successful candidate will synthesise Li/Na ionic conductors, understand and optimise their surface chemistry and then build them into batteries for electrochemical testing. The project will focus on changing variables to improve battery cycling and prevent failure.

### Fabrication of 3D printed gas diffusion electrodes for Li-air batteries

**Peter Bruce**

Design and fabrication of gas-diffusion electrodes, using state of the art micrometer precision 3D printers. Iterative design optimization process linking structural parameters to the electrochemical performance of the battery.

### All natural composites

**Jan Czernuszka**

Composites of calcium salts and natural polymers will be manufactured, characterised and their mechanical properties determined. Calcium salts (e.g. phosphates) are typically sparingly soluble and so can be made to precipitate onto suitable substrates, such as natural polymers – polysaccharides and proteins.

### Dynamic Mechanical Analysis of Natural Tissues

**Jan Czernuszka**

Natural tissues are made up of several proteins and GAGs intricately arranged over several length scales. How these different components interact with each other will be investigated. To complicate matters many tissues have non-isotropic properties that are in themselves size dependent.

### 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. A wide range of materials can be used in conjunction with wet chemical methods and freeze drying techniques to create the aerogel. The voids present in this structure could also be exploited for different purposes, including catalysis, gas adsorption, water purification etc. Alternatively, these voids could also be filled with other material systems/matrix materials to generate multi-functional composite materials.

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.

**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. Otherwise, hot spots from heat accumulation can lead to undesirable consequences such as permanent damage or device efficiency reduction.

One area to target in this field is reduction of the thermal resistance between two mating interfaces so as to improve heat flow, usually from a heat source to heat sink. The materials for this, known as thermal interface materials (TIMS), are usually compliant and fill the air gaps between rough surfaces to increase contact surface area while also providing high thermal conductivity properties.

Electronics packaging also requires multifunctional materials that can protect parts from environmental stressors, both mechanical and chemical. Such materials can be potting compounds, which are poured over an electronic assembly and then hardened. Like thermal interface materials, potting compounds are ideally very good thermal conductors, but should also be electronically insulating to prevent short circuiting of the devices.

In this project, research will be conducted to explore the use of hybrid boron nitride and carbon nanomaterials for use in TIMS 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.

**Synthesis and application of ternary transition metal fluoride nanoparticles on carbon support structures**

**Nicole Grobert**

Transition metal fluorides are a promising class of materials for lithium ion batteries. They exhibit a unique combination of high theoretical capacity and high working potential that makes them ideal for cathode applications. Recently, our lab has developed a new synthesis method for metal fluorides with unprecedented size and shape control. This breakthrough allows for the controlled assembly of ordered electrode architectures and the development of new fundamental insights into the charge/discharge process.

The proposed project will explore the application of this synthesis method and the generation of highly entangled and densely packed carbon nanotube (CNT) support structures using a simple and scalable fabrication technique to generate free-standing CNT composite films with tunable control over film thickness. The proposed project will focus on tailoring the chemistry as well as the structural and electronic properties of these films towards materials systems with even greater potential for lithium ion cathodes. This project is likely to involve engagement with industry partners.

**Designing and testing fibre laminate composites free of carbon fibres for thermal applications**

**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

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

**Nicole Grobert** Co-Supervisor(s): Richard Todd

Nanomaterials are heralded for their outstanding properties as materials of the future yet exploitation of these materials has been limited due to the challenges related to the processing of these materials. 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. This project is likely to involve engagement with industry partners.

**Joints in practical superconductors**

**Chris Grovenor** Co-Supervisor(s): Susie Speller

The large magnets required for applications like medical MRI and large physics experiments like the LHC at CERN are all based on superconductors and all 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 and analytical SEM as well as opportunities to interact with our industrial partners.

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

**Chris Grovenor** Co-Supervisor(s): Susie Speller, Stefanie Zekoll

Thin film sold state batteries are exciting a lot of interest to replace Li-ion batteries with 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. The project will involve film growth and characterisation by SEM/XRD and electrochemical testing.

**Spray casting solid state electrolyte thin films**

**Chris Grovenor** Co-Supervisor(s): Susie Speller, Stefanie Zekoll

Thin film sold state batteries are exciting a lot of interest to replace Li-ion batteries with liquid electrolytes that are heavy and have shown some significant safety problems. This project will explore the use of simple spraying processes for depositing precursor films that can then be crystallised at high temperature to form both electrolyte and electrode films with good uniformity and properties as the basis for a manufacturing process. The project will involve film growth and characterisation by SEM/XRD and electrochemical testing.

**New Zr alloys for fusion applications**

**Chris Grovenor** Co-Supervisor(s): David Armstrong

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 350$^{o}$C. The Zr-V binary system has a very similar phase diagram to Zr-Nb but about 200$^{o}$C higher, and this project will investigate the physical metallurgy of dilute alloys fabricated by arc melting using SEM, XRD and hardness measurements to explore the potential of this alloy system for high temperature applications.

### Scalable HRTEM image simulation of nanoparticles for machine learning dataset generation

**Angus Kirkland**

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.

**Understanding the role of oxide porosity in stress corrosion cracking**

**Sergio Lozano-Perez** Co-Supervisor(s): Chris Grovenor

Stress Corrosion Cracking is a serious environmental degradation problem affecting nuclear reactors. However, cracking behaviour can change substantially between austenitic alloys of different compositions. One of the controlling factors is believed to be the quality of the surface oxide forming when exposed to the reactor cooling water. In this project, you will characterize the quality of the oxide by comparing compositions and paying particular attention to how porous it is. You will use image processing to analyse TEM data and SIMS to understand how porosity facilitates Hydrogen ingress.

**Cracks in heterogeneous materials, quantified in 3D by in situ X-ray tomography and Digital Volume Correlation**

**James Marrow** Co-Supervisor(s):Yang Chen

Micro-cracking is an important characteristic of brittle and quasi-brittle materials, and it can be controlled to improve their fracture resistance. However. new methods are needed to quantify cracks (particularly their opening and surface area), in order to provide feedback to models used in the design of innovative, tougher materials.

This project asks the question "How can cracks at the limits of experimental resolution be detected and quantified?". A novel image subtraction technique to study crack development, based on Digital Volume Correlation of high resolution X-ray tomographs, is being implemented in MATLAB to measure the crack opening and surface area in damage networks (following the method of https://hal.archives-ouvertes.fr/hal-01593058). You will optimise and further develop this code, and then apply it to recent in situ synchrotron X-ray tomography studies of fracture and fatigue of advanced ceramic matrix composites and a model cast iron. You will design and conduct validation tests of the crack quantification method, using in situ laboratory X-ray tomography experiments on model materials. There are opportunities for image-based modelling using finite element or/and Fourier transform based methods if you are interested in this aspect, although this is not essential for a successful project.

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

**James Marrow** Co-Supervisor(s): Nicola Pugno (Trente University

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.

**Fracture of Novel Graphites for Next Generation Nuclear Energy**

**James Marrow**

There is a need to measure the fracture toughness and resistance to stress concentrating notches in fine grained nuclear graphites that are the proposed structural materials for next generation high temperature and molten salt nuclear fission reactors. These graphites will be exposed to irradiation, oxidation and corrosion and cannot be replaced during the reactor life. Materials test reactors are used to provide accelerated irradiation tests to qualify and select materials, but there are severe restrictions imposed on the sample dimensions. Hence there is to test small specimens to measure properties.

A novel method has been developed to evaluate the stress intensity factor by using optical digital image correlation (DIC) to measure displacement field around the crack tip (http://dx.doi.org/10.1007/s11340-017-0275-1). A recent Part II project (Georgina Mordue, 2017-18) demonstrated this could be applied to measure the fracture toughness of a nuclear graphite.

This project asks the question “What is the effect of graphite microstructure on the fracture toughness?”. This experimental study will use optical DIC to measure, in situ, the displacement fields of a centre-hole notched compression specimens during crack propagation tests. The elastic properties and fracture toughness will be evaluated from these data. The effects of thermal oxidation on the graphite microstructure will be examined, using computed X-ray tomography, and the effects of oxidation on the elastic properties and toughness will be investigated. The analysis will require some use of finite element modelling methods, and also post-processing of data using tools written in MATLAB.

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### Investigating nanoscale solute cluster formation mechanisms in high-strength aluminium alloys by atom probe tomography

**Michael Moody** Co-Supervisor(s): Paul Bagot

Novel fabrication routes are under development to produce high strength light-weight aluminium alloys for automotive applications to improve levels of energy absorption upon impact. However, there is a lack of fundamental understanding of how the desired microstructure develops. Atom probe tomography has a unique ability to visualize and quantify the size and chemistry at the initial stages of atomic-scale solute clustering, which is essential to understand the impact of each processing stage on the final microstructure. This project aims to identify the effects of trace alloy additions on the cluster formation, and explore the impact of various processing parameters on the clustering kinetics.

### Mapping strain by electron diffraction and imaging

**Pete Nellist**

Strain plays a hugely important role in Materials Science, ranging from controlling the interaction of dislocations to the catalytic activity of alloyed nanoparticles. Measuring strain at high spatial resolutions is an important characterisation challenge. Both electron imaging and diffraction methods can be used, but how a strain that varies through the thickness of a sample affects these measurements has not been extensively studied. The project could be purely modelling, or contain a combination of modelling and electron microscope experiments. The materials systems to be studied may include alloyed nanoparticles for hydrogen fuel cells, or dislocations in fusion reactor materials.

### Understanding Screw Dislocation Structures in BCC metals

**Pete Nellist** Co-Supervisor(s): Dave Armstrong

BCC metals (including iron, tungsten, chromium and vanadium) are key candidate materials for structural applications in future fusion reactors. Their mechanical properties are largely controlled by the relatively immobile screw dislocations. Whilst the exact reason for this is known to relate to the detailed atomic arrangement at the core of the dislocation, but a full 3D characterisation of such defects has not before been possible.

This project will perform simple, controlled mechanical tests at a range of temperatures on a BCC metal (exact metal will be chosen nearer the time) to produce well defined arrays of dislocations. A preparation method will be refined to allow these to be captured in a single TEM foil. We will then make use of a novel "optical sectioning" procedure we have developed in our laboratory to determine the structure of dislocations at atomic resolution in 3D using electron microscopy allowing the detailed atomic arangement of the dislocation to be fully resolved. The project will make use of mechanical testing, SEM-EBSD and TEM and also include data analysis in MATLAB.

### Modelling the imaging of bonding in materials by combining electron microscopy with density functional theory

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

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

### Batteries for grid-scale energy storage

**Mauro Pasta**

New types of energy storage are needed in conjunction with the deployment of solar, wind, and other volatile renewable energy sources and their integration with the electrical grid. No existing energy storage technology can provide the power, cycle life, and energy efficiency needed to respond to the costly short-term transients that arise from renewables and other aspects of grid operation. We are currently working on a new family of insertion electrodes based on the Prussian Blue open-framework crystal structure. This structure is fundamentally different from other insertion electrode materials because of its large channels and interstices.

It is composed of a face-centered cubic framework of transition metal cations where each cation is octahedrally coordinated to hexacyanometallate groups and has wide channels between the A sites, allowing rapid insertion and removal of sodium, potassium and other ions. In addition, there is little lattice strain during cycling because the A sites are larger than the ions that are inserted and removed from them. The result is an extremely stable electrode: over 40,000 deep discharge cycles were demonstrated in the case of the copper hexacyanoferrate cathode.

The student will work on synthesizing new open-framework materials, perform an in-depth structural characterization and evaluate their electrochemical properties.

### Laser written qubits in wide band gap crystals

**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 carrying out some first experiments on the generation and characterisation of colour centres in such materials using laser processing methods, and evaluation of their optical and spin properties for use in quantum technologies.

### Measuring atmospheric aerosols with microcavity sensors

**Jason Smith**

Atmospheric aerosols are of critical importance in both human health and environmental contexts, and new devices to monitor levels and characteristics of aerosols are of growing importance. This project will involve the testing of a new analytic instrument that has been developed by the group for nanoparticle analysis to measure aerosols. The instrument is based on optical microcavities and the goal of the project will be to inject aerosols into these sensors, detect their presence and measure their size and composition.

You will work with other group members focused on related topics and with engineers from our recent spinout company Oxford HighQ Ltd which is currently commercialising the instruments for characterising nanoparticle in fluids.

**Triggered single photon sources based on point defects in solids**

**Jason Smith**

Devices which produce single photons of light on-demand are expected to be a key component of quantum technologies, offering a range of applications in secure telecommunications, metrology and sensing. At the core of these devices is an atom-like system in a material, and much research is currently being carried out to identify and optimise candidate systems, with the very first examples now coming to market. This project involves exploring the properties of novel point defects in wide band gap materials (diamond, SiC, hBN) as potential room temperature single photon sources. The project will contribute to the wider efforts of the team within the Photonic Nanomaterials Group working on this topic.

**Microstructure of MgB2 bulk magnets**

**Susie Speller** Co-Supervisor(s): Chris Grovenor

Magnesium diboride is an interesting superconducting material for applications in cheap, 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 presses that give unique microstructures in these ceramics.  This project will use a variety of XRD and SEM techniques to study these samples processed under a wide range of different conditions to understand the relationship between microstructure and properties.

**Nacre-like alumina ceramics**

**Richard Todd** Co-Supervisor(s): Nicole Grobert

Sea shells are made from calcium carbonate plates interleaved with a soft biopolymer. Their mechanical properties are very much better than either material alone. The question behind this project is: could a really tough ceramic be made using better base materials combined with the same microstructure?

The aim is to use commercial alumina platelets bonded with a variety of weaker phases to investigate the possibilities. The project will involve ceramic processing, SEM and mechanical testing.

**Synthesis of 2D materials by chemical vapour deposition**

**Jamie Warner**

This project will involve growing large area monolayer 2D crystals by chemical vapour deposition. It will involve the growth of semiconducting 2D materials such as MoS2, WS2, and semi-metal 2D materials of graphene, and insulating hBN monolayers. New 2D materials will also be explored. The work involves using powder precursors to create vapours in the gas phase that react on the surface of substrates to grow 2D crystals as monolayer polycrystalline films.
The challenges involve growing larger domain sizes, uniform monolayer thickness control, and the ability to transfer the material off the growth substrate onto another substrate to build vertical heterostructure stacks. The project will use optical microscopy to image the 2D Materials, some SEM to also visualize the materials, and PL/Raman spectroscopy to characterize the structure. The materials are used in electronic and opto-electronic devices, and in some cases for electrochemical catalysis. The project will be integrated with other members of the group to take materials from synthesis, to characterization and nanoelectronics device fabrication. The aim is to create new classes of flexible ultrathin transparent electronic devices that form the basic components of photodetectors and light emitting devices.

**Dislocation Loops in Irradiated Metals – effects on diffraction peak broadening**

**Angus J Wilkinson** Co-Supervisor(s): Ed Tarleton

Irradiation of metals by fast neutrons, or ions causes undesired hardening and a loss of ductility through the generation of many small dislocation loops. Transmission electron microscopy can be used to image the loops directly and quantifying loop density and size distributions is possible but laborious. The lattice strain fields caused by the loops also affect the width of peaks seen in X-ray (and neutron) diffraction data, and offers a potentially quicker route to quantifying the average loop density over large material volumes. Direct comparisons loop densities determined by TEM and X-ray peak broadening show large disagreements.

This project will address a potentially very poor approximation made in the analysis of X-ray peak broadening for loop density. To date, analyses have all been based on approximating the loops a set of straight dislocation lines of infinite extent; which is clearly incorrect. We will use DDLab, a MATLAB-based dislocation dynamics code, to calculate the spatial distributions of lattice strains close to dislocation loops and compare to the isolated straight line case. We will determine the effects of loop size, loop shape and loop density on the peak broadening. The analysis may also be used in interpretation of HR-EBSD strain measurements, and/or electron channeling contrast imaging of irradiated materials.

### Fatigue crack initiation in austenitic stainless steels

**Angus J Wilkinson** Co-Supervisor(s): 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. In the high cycle regime, the macroscopic behaviour of the sample is essentially linear elastic. However, there is some micro-plasticity but it is highly localised. Understanding, where this plasticity occurs in the microstructure is important for development of improved alloys and heat treatments. This project will use a novel ultrasonic (20 kHz) testing method, developed by the group and capable of applying a high number of cycles in a short timeframe to small sample volumes spanning a few 100 microns. The study will centre on 304 stainless steel and aim to characterise microstructural features at sites of local plasticity and short fatigue cracks using advanced techniques such as HR-EBSD, electron channelling contrast imaging and possibly AFM.

### Nano-scratch testing: Understanding fundamentals of wear

**Angus J 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 whereby the sliding contact of single asperities can be simulated in controlled experiments. Investigation of the influence of grain boundaries and crystallographic orientation of materials will enable the wear processes to be further understood.

In this part II project, nanoscratch experiments will be carried out on polycrystalline Cu (FCC) and Fe-Cr (BCC). The influence of grain size, and grain boundaries on the nanoscratch response of these materials will be studied by performing nanoscratch experiments up to, and across grain boundaries. The effect of crystal orientation on the scratch response will be investigated as the scratch passes through a grain boundary into a grain of different orientation. 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. In situ lift outs of cross sections through the scratch track will be made using FIB, and HR-EBSD will be used to map the subsurface deformation of these experiments.

### Novel Texturing Processes for Silicon Photovoltaics manufacturing

**Peter Wilshaw** Co-Supervisor(s): Sebastian Bonilla

In order to move to a low-carbon future, and avoid the worst effects of anthropogenic climate change, continuing reductions in the cost of renewable energy are required. The Semiconductor Group at Oxford Materials, in collaboration with international research partners at Fraunhofer ISE in Germany and the University of New South Wales in Australia as well as industry partners, is working to reduce the cost of photovoltaic cells. Part II students would work as part of a dedicated group of researchers on state-of-the-art techniques for improving the performance of crystalline silicon solar cells, which account for over 90% of all currently manufactured solar cells. Texturing of silicon wafers for solar cell production has been an ongoing concern for cell manufacturers. While anisotropic texturing of mono-crystalline silicon can reduce the weighted average reflection (WAR) of bare silicon to below 10%, most approaches on multicrystalline materials yield WAR's in excess of 25%. Furthermore the traditional approach of using acidic etching solutions to preferentially attack defect sites is incompatible with new wafer sawing techniques.

In this project the Part II Student will evaluate novel texturing approaches for silicon involving liquid and gas-phase etching. If successful this technology will reduce the cost of solar electricity by realizing superior optical performance with a reduced cost of production.

### New surface passivation processes for silicon solar cells

**Peter Wilshaw** Co-Supervisor(s): Sebastian Bonilla

Silicon photovoltaics is a key technology to provide the world with renewable, inexpensive and reliable energy. Efficiency in silicon solar cells is partly limited by recombination of photo-excited electron-hole pairs at surfaces and interfaces. Future generations of high efficiency solar cells require cheap techniques for producing semiconductor/dielectric interfaces with very low recombination. This process is called surface passivation and the development of efficient new processes is critical to the development of next generation solar cells. Existing work in the semiconductor group has produced some of the world's best passivated silicon surfaces. The problem we have is that, at present, the passivation we produce is not stable over a period of years as required for practical cells.

This project aims to develop a technique for stabilising the passivation effect and will involve controlled modification of surface dielectric films deposited on the cells. The student performing the work will be involved in deposition of standard and modified dielectrics using semiconductor facilities and characterisation of their properties using electronic techniques. We expect that by correlating passivation performance with the details of the dielectrics produced we will be able to produce stable passivation.

### Using DFT to interpret spectra from atomic vibrations in the electron microscope

**Jonathan Yates** Co-Supervisor(s): Rebecca Nicholls

Recent advances in electron microscopes mean that it is now possible to combine atomic resolution imaging with high resolution spectra showing bond vibrations. These spectra provide information about chemical, electronic and catalytic properties of materials. Interpreting the spectra obtained is not trivial. This project will use Density Functional Theory calculations running on supercomputers to interpret and inform experimental studies of nanoscale vibrations. Several areas could be studied including defects in nanostructures and pharmaceutical polymorphs.

**DFT modelling of the effect of carbon additions on grain boundary toughness in alumina**

**Jonathan Yates** Co-Supervisor(s): Richard Todd

We have recently found that the addition of just 0.01% carbon to alumina doubles the grain boundary toughness, resulting in substantial property improvements. This may be a direct effect of C on the g.b. structure or an indirect effect of impurity removal (e.g. silica) by carbothermal reduction. This project aims to use Density Functional Theory to model alumina grain boundaries with small amounts of doping (carbon, impurities) to investigate these and other possible explanations for this striking effect.

**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.

**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.