DEPARTMENT OF MATERIALS

PART II PROJECTS

2021/2022

UNDERGRADUATE PART II PROJECTS

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

Further projects may be publicised at a later date.

There will be an open afternoon on Thursday 25th February 2021 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 2021.

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PROJECTS ON OFFER:

1. 3D-cavity detection of mechanical motion

Natalia Ares Co-Supervisor(s): Andrew Briggs

Superconducting 3D cavities allow us to gain exquisite control of the vibrations of nanometer thin membranes. The aim of this project is to optimize the interaction of cavity photons 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 superconducting circuits and nanoscale motion.

2. Radio-frequency circuits for quantum device readout

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

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

3. Developing a flexible control interface for quantum experiments

Natalia Ares Co-Supervisor(s): Andrew Briggs

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

4. Sustainable High-Entropy Alloys

David Armstrong Co-Supervisor(s): Angus Wilkinson

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 their high configuration entropy and severe lattice distortion, HEAs possess outstanding mechanical performance even under extreme environment. Due to their variable composition they may be an attractive alloy system to reuse scrap or waste metals to produce materials suitable for demanding applications, with low environmental impact. Alloys will be manufactured from common scrap materials with a particular aim to find alloy compositions tolerant of containing both iron and aluminum. Alloys will be produced using arc melting and microstructures studied using XRD and SEM-EBSD and SEM-EDX. Mechanical properties of the best alloys maybe studied using nanoindentation and 4-bending. Outcomes of the mechanical testing/characterisation will be used to provide manufacturing guidelines for the alloy processing group in Oxford. Strong interactions will be made with both UK/USA collaborating universities.

5. Advancements towards high energy density solid state batteries

David Armstrong Co-Supervisor(s): Ed Darnbrough

The key challenge around realising the potential of all solid state batteries (SSB) is the workable thickness of the electrolyte. Current materials have short cycling lifetimes due to poor mechanical properties which stem from inhomogeneities and porosity created by the production route. In this project you will be working to understand the role of density and internal surfaces on the mechanical properties of solid electrolyte materials, via powder compression with in-situ conductivity measurements and microscale bend testing of new materials comparing the latest production routes. The results from this will allow us to minimise the electrolyte thickness in a SSB increasing the energy density. This is a fundamental link into the considerable solid state battery research that is already being conducted in the department.

6. Stress evolution during cycling of solid state batteries

David Armstrong Co-Supervisor(s): Ed Darnbrough

All solid state batteries suggest a future of smaller, lighter and higher capacity mobile energy sources to help democratise the electricity availability across the globe. With this new technology comes new challenges and questions, primarily around volume transport and change within the battery during cycling. This project would look to utilise new capability within the department to monitor the changes within an all solid state battery as a whole considering the changing stresses within each component (anode, electrolyte and cathode) during cycling. You will marry this experimental data with simple modelling to unpick the roles of the different materials involved. This work will elucidate many questions on the underlying mechanism that drive different failure modes and how the application of external pressure in different orientations can hope to suppress them.

7. Nanostructured alloys for next generation nuclear reactors

David Armstrong Co-Supervisor(s): Hazel Gardner, Michael Moody

Materials used in nuclear reactors must often withstand extreme environments. Material requirements can include a combination of good high temperature performance, irradiation resistance and corrosion resistance. Nanoscale material design is key to ensure materials meet these challenging criteria. Examples of nanostructured alloys include high entropy alloys for fusion reactors and nickel-based oxide dispersion strengthened alloys for molten salt fission reactors. High-resolution characterisation is needed to inform the design, development, and optimisation of these alloys.

In this project, new nanostructured alloys that are being developed in the Department will be analysed using 3D nanoscale atom probe tomography (APT). APT samples will be prepared by the electropolishing method. Complementary indentation will link APT microstructural analysis and chemical information to mechanical properties. Outcomes of the project will be used to inform further materials processing.

8. Deformation and Interfacial failure mechanisms in polymer films

David Armstrong Co-Supervisor(s): Hazel Assender

We have used various forms of radiation curing (UV, electron-beam, plasma) to polymerize diacrylate monomers to a solid, crosslinked polymer layer for coatings in functional materials and devices. Experimental data suggest that the degree of cure depends on the amount of radiation, but also the time it is applied and the depth of material. This project will use micro-mechanical testing methods developed in Oxford for measuring the mechanical properties of these layers and the interfacial adhesion properties. This will involve high speed mechanical mapping of the samples allowing for statistically significant data sets to be produced. This data will be linked to bulk mechanical data of the coatings and used to understand how the curing process effects mechanical properties.

9. Liquid lithium corrosion of materials for nuclear fusion

David Armstrong Co-Supervisor(s): Chris Grovenor

For nuclear fusion to be a commercial reality reactors must be self-sufficient in tritium. The only viable route for lithium production is through the capture of a neutron by a lithium atom which through decay produces a helium and a tritium atom. There are two main tritium breeding concepts, solid and liquid breeders. Liquid breeders use large volumes of flowing liquid lithium or lithium-lead eutectic alloy to capture neutrons and produce tritium. This has the advantage that tritium can be easily extracted and the liquid is not subject to irradiation damage as in solid breeders. However the major disadvantage is the corrosive nature of liquid lithium limits the alloys that the vessel can be made from. Currently a range of steels, zirconium alloys and vanadium alloys have been suggested but few trials of liquid lithium corrosion have been carried out. This project will perform liquid lithium corrosion inside a glove box, at a range of temperatures on alloys of interest to the fusion community. Samples will be examined using optical microscopy, scanning electron microscopy, EBSD and EDX. The aims will be to find alloys with good corrosion resistance, understand what corrosion products are produced and investigate the effect of different microstructures on corrosion resistance. This will then be fed back into ongoing alloy design projects.

10. Microchannel Electrodes for Implantable Neuronal Interfaces

Hazel Assender

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

11. Nanostructured alloys for next generation nuclear reactors

Paul Bagot Co-Supervisor(s): Hazel Gardner, David Armstrong

Many materials for safety critical components to withstand the extreme environments fusion and fission reactors must be designed at the atomic-scale. Hence high resolution characterisation is a critical step in alloy design and the development of processing routes to optimise these materials. In the Materials Department we are developing high entropy alloys for fusion reactors and nanostructured nickel based ODS alloys for molten salt fission reactors.
In this project, 3D nanoscale atom probe tomography analyses will be used to characterise the new materials and inform the next iteratiion of processing steps.

12. Predicting the performance and usefulness of near-term quantum computers

Simon Benjamin

Quantum computer prototypes are reaching the point that they are interesting beyond being physics experiments. For example, in 2019 Google announced a 53 qubit device, which is sufficiently large that no conventional computer can predict its behaviour and in 2020 a Chinese team presented a similar result. However, the question of whether such machines can be useful for anything is still undecided; because each elementary operation, or ‘gate’ in the machine is imperfect, with up to 1% noise, the output after many gate operations is very noisy and imperfect. All such devices are called NISQ for Noisy Intermediate Scale Quantum systems.

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

The project will include these themes:

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

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

13. New materials for on-chip optoelectronic computing

Harish Bhaskaran Co-Supervisor(s): Wen Zhou

The part II student will join a thriving research group to pursue new materials investigation for a range of exciting applications in neuromorphic and cognitive computing applications that integrate light onto silicon chips.

14. Novel electro-optical approaches to digital-to-analogue conversions for AI applications

Harish Bhaskaran Co-Supervisor(s): Johannes Feldmann

The energy efficiency, speed and precision of neuromorphic analogue photonic processors is often limited by the interface with the electronic world, namely digital-to-analogue (DAC) and analogue-to-digital (ADC) conversions. Therefore, the project will include the development, fabrication and measurement of new approaches to these conversions based on both mixed electro-optic and also all-optical techniques. The student will join a thriving research group at the forefront of integrated photonic computing and help integrating the developed DACs and ADCs with existing and new unconventional optical processors to solve demanding tasks in artificial intelligence applications.

15. Engineering research and development for a new display technology – Industry Project

Harish Bhaskaran

This is a project to be held at an Oxford University spin-out, Bodle Technologies, based at Begbroke Science Park in conjunction with the Advanced nanoscale Engineering Group in the Department of Materials. This will be supervised by an engineer/VP at Bodle and by HB.

The specific project would depend on the technology development stage at the time the student starts as it would be oriented to be relevant to the priorities at the time. Broadly it could involve developing innovative processes, material or test methodology to advance the development of SSRD at either the individual pixel or matrix level.

It could involve work in a clean room on photoresist processes, Reactive Ion Etching, PECVD or ALD, sputtering of complex stacks involving phase change chalcogenide materials, work with developing high tech electro-optical test equipment, improving finite element modelling and matching to experiments or development of colour measurement equipment.

Contact: andrew@bodletechnologies.com

16. Efficient design and optimisation of bio-photonic sensors

Harish Bhaskaran Co-Supervisor(s): Mengyun Wang

Optical biosensors possess significant competitive advantages relative to other approaches and their intrinsic versatility has facilitated their use for rapid, simple, and cost-effective detection of molecular markers. Though many innovative technologies have been proposed to realize optical biosensors with improved performance in the past few years, the widely recognized potential impact of optical biosensors remains largely unexpressed and the state-of-the-art bio-photonic sensors are far from a practical application. Thus, further effort through an interdisciplinary platform is of great interest. In this project, the student will join an extremely promising research on bio-photonic sensors, including novel design of bio-photonic structures, innovations in fabrication strategies, and corresponding emerging photonic-related bio-sensing applications.

17. The quantum properties of metal centres in graphene via pulsed EPR spectroscopy

Lapo Bogani Co-Supervisor(s): Michael Slota

Graphene is a material with amazing structural, conducting and mechanical properties. On the other hand, it is still difficult to add one property to it: a magnetic behaviour. This is because graphene is, by itself, diamagnetic. We could recently introduce spin states into synthetic graphene nanostructures by chemical functionalization (Nature 2018) and topological manipulation (Science 2019). On the other hand, one ingredient remains missing: a sizeable spin-orbit coupling, which would allow mixing electronic and spin states so as to create truly multifunctional topological materials. In this project you will investigate our next generation of graphene materials, where metal centres with high spin-obit coupling have been introduced. You will measure the quantum and classical spin properties using advanced pulsed electron paramagnetic resonance techniques, and interpret the results. In this project you will learn the basics of quantum information, advanced pulse techniques for their implementation, and the relevant data treatment. This is a project aimed at a student interested in learning advanced instrumentation, where most of the time will be spent on data acquisition and treatment.

18. Optimizing cantilever torque magnetometers

Lapo Bogani

The technology of cantilever-torque magnetometry has now been around since several decades, and is widespread in science and technology. Scientific instruments, and the magnetometers operating at the highest achievable fields rely cantilever torquemeters working at cryogenic temperatures. In this project you will push the current limits in how cantilever torque meters can be operated, in order to produce state-of-the-art scientific instrumentation.
This is a very hands-on project, designed for a student who wants to see the reality of laboratory work. You will learn how to design (e.g. using CAD), model (e.g. using fine element methods) and operate cantilever torque devices, how to cool them down to cryogenic temperatures, and how to interface scientific equipment. You will test what characteristics allow for optimal performance, and eventually you will use the setup developed to measure samples of molecular magnetic materials.

19. Single-molecule Spin Spectroscopy

Lapo Bogani

One of the fundamental challenges of contemporary science is to be able to probe the behaviour of single atoms or molecules: investigating a single quantum system allows probing the interaction with the environment on the quantum behaviour, and testing our understanding of fundamental phenomena. The spin energy levels of a molecule are usually investigated by shining microwaves, so that the changes in reflectivity of a resonator is measured while a magnetic field is applied. This project will test a completely different approach, in order to reach single-molecule sensitivity: the molecular states will be probed by single-electron-transport, while sending microwaves through the electrodes. In doing so, you will combine the techniques of single-molecule transport and electron paramagnetic resonance. You will have the possibility of learning nanofabrication, nanoelectronics, microwave optics, and cryogenics. You will test what device geometries allow for optimal performance, and **e**ventually you will use the setup developed to measure samples of molecular magnetic materials.

20. Advanced Metallisation Technology for Next-Generation Photovoltaics

Sebastian Bonilla Co-Supervisor(s): Peter Wilshaw

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

This project aims to explore novel contact and metallisation technologies that can address this critical hurdle for the future of solar electricity generation, using solvo-dynamic printed nanowire high aspect ratio contact electrodes. Silver-free metal to semiconductor contacts will be explored in collaboration with our international partners, and new technologies will be proposed to achieve low-cost manufacturing of efficient metallisation for single and multijunction solar cells.

This project requires hands-on electrical and optical measurements of materials, as well as data processing and analysis. Analytical and electrical characterisation techniques will be used to assess the performance of the metallisation, including advanced nano scale mass-spectroscopy and electrical current transport. The understanding and development from this project will result in improved manufacturing of commercial solar panels, which in turn will help mitigate the devastating consequences of climate change.

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

Sebastian Bonilla Co-Supervisor(s): Peter Wilshaw

Ion charged dielectrics are a class of thin-film material that possess a permanent charge. The charge storage capability of these materials makes them essential to a wide range of applications, from telecommunications to air filters and biomedical devices. At Oxford Materials, we have developed new methods to produce substantial concentrations of charge in dielectric thin films, in to fully exploit their potential in making of devices.

This project aims to discover new dielectric-ion combinations and apply them to the manufacture of optoelectronic devices, like solar cells, photodetectors, and photodiodes. The project will involve establishing a reproducible and controllable method of growing nanometre scale thin films using different synthesis methods, followed by delivery of new precursor ions, and their drive in into the dielectric. After the methodology is stablished the novel ion-charged dielectric systems can be integrated into devices, and their performance will need to be characterised.

This project requires hands-on electrical and optical measurements of materials, as well as data processing, analysis, and modelling of the observed current transport characteristics. Ultrathin dielectric films will be employed in the next generation of silicon solar cells to produce architectures with minimum losses. As such this project feed in the Lab's aim of improving future photovoltaics technology to help accelerate the green energy transition.

22. Spin-on Doping and Laser Contacting Tunnelling Electron Contacts for High Efficiency Solar Cells

Sebastian Bonilla Co-Supervisor(s): Peter Wilshaw

While conventional silicon solar cells are a strong technology, an overwhelming drawback is the use of very high doping in contacts and carrier separation layers. This prevents further increases in their power conversion efficiencies. Passivating carrier-selective contacts have been recently demonstrated using thin films. These materials can allow cell architectures that overcome the drawbacks of current technologies, and are potentially much more cost effective.

In this project we aim to study and develop tunnelling oxide passivating selective contacts that are based on spin-on doping and laser contacting of amorphous silicon layers. The project will involve the development and synthesis of phosphorous spin-on doped layers using our Semiconductor fabrication facilities at the Materials Department.

This project requires hands-on laboratory synthesis of materials, electrical and optical measurements of devices, as well as data processing and analysis. This project integrates into the Lab's global aim to boost the future reductions in the cost of solar energy, which are required in the world to move to low-carbon electricity generation, and avoid the worst effects of anthropogenic climate change.

23. DFT modelling of O-redox cathode materials

Peter Bruce

Lithium-ion batteries have revolutionised portable electronics and the demand continues to grow as transport is electrified. The cathode represents one of the greatest barriers to increasing the energy density of Li-ion batteries. In current cathode materials Li removal during charge is compensated by transition metal oxidation, limiting energy density. A new class of high voltage materials stores charge on both the transition metals and oxide anions, potentially offering a 50% increase in energy density.

However several problems prevent their application, including structural changes, oxygen loss, slow kinetics and capacity fade. This project will use DFT to investigate the changes taking place in these cathode materials during cycling. This will help to provide valuable insight into the processes underpinning anionic redox.

24. Calcium carbonate to calcium phosphate transformations

Jan Czernuszka

Calcium phosphates are useful in osteogenic augmentation devices and in water purification systems. This project aims to turn naturally occurring calcium carbonates into more useful calcium phosphates.

There are a family of calcium phosphates and they can be formed under specific conditions. The product will be analysed using the Depts macro and micro analytical and structural techniques.

25. New materials for quantum device architectures

Marina Galano Co-Supervisor(s): Natalia Ares, Fernando Audebert

New materials can open exciting new possibilities for quantum devices, which are the object of significant investments worldwide with the aim of developing new quantum technologies. The aim of this project is to optimize the fabrication methods for solid-state quantum devices by improving the properties of the electrodes. The project is likely to be of interest to those students that enjoy quantum technologies and material science..

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

Jicheng Gong Co-Supervisor(s): Angus Wilkinson

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

This project will investigate the influence of the testing rate (strain rate) on HCF crack initiation and short crack growth in titanium alloys by comparing the ultra-small & ultra-fast fatigue test with a low frequency meso-cantilever test. Two SN curves will be achieved. In-situ, intermittent and post-mortem analysis by SEM and EBSD characterisation will be conducted to underpin the fatigue behaviour and properties as a function of the strain rate.

Static meso-cantilevers can be deflected by the nanoindenter to measure the load-displacement response. Strain rate jump tests and DIC analysis will be performed in these static meso-cantilevers to establish the correlations between the strain rate and plastic deformation with respect to the microstructure. The results will be used to interpret the effect of strain rate on HCF fatigue.

Finite element model will be implemented to simulate the dynamic response of a cantilever and calculate the stress in an ultrasonic fatigue test.

27. 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.

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

29. 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.

30. 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.

31. 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.

32. Solid state batteries based on thin film electrolytes

Chris Grovenor Co-Supervisor(s): Susie Speller

Thin film sold state batteries are exciting a lot of interest to replace normal Li-ion batteries containing liquid electrolytes that are heavy and have shown some significant safety problems. Previous Part II projects have developed a reliable process to deposit LiAlGePO(N) thin films with good properties, and this project will take the next step towards fabricating and testing all thin film battery structures. The project will involve film growth, careful characterisation by SEM/XRD and the electrochemical testing of prototype batteries.

33. Li alloys for solid state batteries

Chris Grovenor

Storing the highest energy densities in solid state Li batteries requires the use of metallic Li as the anode, but Li metal is very soft, extraordinarily reactive and difficult to use in practical devices. One idea that is being explored to improve the properties is the formation of high Li content alloys, and the simple Li-Mg binary system has been most studied to date. This project will make and test novel ternary alloys in which the microstructure/mechanical properties and electrochemical performance can be controlled independently.

34. Persistent joints in high temperature superconductors

Chris Grovenor Co-Supervisor(s): Susie Speller

The large magnets required for applications in medical MRI and large physics experiments like the LHC at CERN are all based on superconductors, and can contain numerous joints that are often the (very expensive) points of failure.
This project will work with Oxford Instruments on making and testing joints in Bi-2212 superconducting wires – how to improve reliability and performance, and understanding what goes wrong. The project will involve improving our joint making processes, using XRD and analytical SEM to check phase purity and microstructure of the joints, and measuring the persistent performance of small coils.

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

Angus Kirkland Co-Supervisor(s): Chen Huang

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

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

36. Atomic resolution electric field mapping

Angus Kirkland Co-Supervisor(s): Christopher Allen

Due to the dimensional constrains of a nano-electronic device, any deviation from a perfect crystal lattice can have profound consequences on its electronic characteristics. These deviations can take the form of defects in the crystal lattice, substitutional/interstitial dopant atoms, or edge/surface structure. Modern transmission electron microscopes (TEM) have made imaging the atomic structure of a wide range of nano-materials fairly routine. From this experimentally determined atomic structure the theoretical internal electric fields can be calculated and electronic characteristics predicted. Recent advances in TEM detector technology now enable the direct imaging of internal electro-magnetic fields in nano-materials at atomic resolution. To achieve this an electron probe is focused onto the sample surface in a standard scanning-TEM (STEM) experiment and the far-field diffraction pattern recorded at each electron probe position. Any deflection in the forward scattered bright field disk is related to a momentum transfer from the internal electro-magnetic field of the material to the electrons in the probe. By measuring changes in the intensity distribution of the bright field disk in the recorded diffraction patterns the internal electric field of the material can be calculated. In general these experiments are performed at a reasonable high electron dose in order to ensure good signal to noise ratio in the recorded diffraction patterns. However this high electron dose transfers significant energy to the sample and can cause bond breaking and atom ejection changing the very atomic structure being investigated.

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

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

37. Lightweight High Entropy Alloys

Enzo Liotti

High entropy alloy is a term applied to a relatively new type of metallic alloy system that comprises near equiatomic concentrations of at least three or more alloying elements. A surprising characteristic of HEAs is that despite their apparent compositional complexity, they comprise usually a complete or near simple solid solution. Since their discovery simultaneously in Oxford and Japan in 2004 a large number of these alloys have been manufactured at small scale and their structure and properties reported in the scientific literature. Technologically, the alloys are immature - but some data shows intriguing and attractive combinations of properties, such as ultra-high toughness at cryogenic temperatures.

The project will focus on a selected number of lightweight high entropy alloys (HEAs) processed from powders to bulk using field assisted sintering technique (FAST) or cast from the liquid to produce near-net shape components. The property assessment will focus on the characterization of the microstructure and how to manipulate the processing parameters to enhance performance. The work will involve the use of SEM, with both EDS and EBSD and X-ray diffraction XRD.

38. Optimizing SIMS mapping of nuclear materials

Sergio Lozano-Perez Co-supervisor(s): Gareth Hughes and Junliang Liu

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

39. In situ 3D study of damage mechanisms in novel SiC-SiC ceramic composites for aerospace applications

James Marrow

Ceramic composites have the potential to expand the temperature limits of critical components in aerospace applications, and various novel methods to efficiently manufacture these materials are in development (https://doi.org/10.1016/j.ceramint.2018.12.020).
A critical step is the formation of the SiC matrix within the fibre lay-up, and the processes being considered include PIP (polymer infiltration processing) and LSI (liquid silicon infiltration). These result in quite different microstructures (porosity, fibre coatings, residual thermal strains) with potentially important consequences for their mechanical properties, including the ability to accommodate deformation.

This project, in collaboration with DLR (German Aerospace Centre), asks the question “how do SiC composites, prepared by PIP and LSI, accommodate strain within their microstructures?” This will be done by in situ X-ray tomography, analysed by digital volume correlation, to quantify the relation between micro mechanical damage and macroscopic properties (i.e. increased elastic compliance with micro cracking). The effect of loading direction relative to the fibre architecture will also be studied. The project will involve mechanical testing, computed tomography, data visualisation and numerical analysis by image correlation, with opportunities to apply finite element simulation.

40. Indentation Damage in Advanced Ceramics and Composites

James Marrow

Indentation damage in ceramics is a complex process that includes elastic and inelastic deformation as well as brittle fracture (http://dx.doi.org/10.1016/j.jeurceramsoc.2014.04.002). It forms the basis of several standard tests for measuring the mechanical properties of ceramics and is also highly relevant to practical applications such as light weight armour and the wear of high temperature cutting tools. However, the details are still not well understood, which impedes the design of damage resistant ceramics and composites. This is partly because it is very difficult to study the processes that occur under the indention. One method for studying the internal structure of materials is X-ray computed tomography (XCT), which can be applied with sub-micron resolution to materials that are opaque to visible light; the obtained 3D datasets can be analysed by digital volume correlation methods (DVC) to measure the full field displacements that arise from damage and cracking.

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

41. 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 materia .
You will design experiments to study the deformation and failure of CNTT materials, using in situ, high resolution computed X-ray tomography. Deformation and fracture will be quantified using digital volume correlation, as a function of the applied strain. The project will involve mechanical testing, computed tomography, data visualisation and numerical analysis (Matlab), with opportunities to apply finite element simulation.

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

James Marrow

Salt contamination on the surfaces of stainless steel components can develop very high concentrations of chloride ions under certain combinations of humidity and temperature. This can create the conditions for pitting corrosion (http://dx.doi.org/10.1149/1.3407553). The pits are stress concentrations, from which stress corrosion cracks may initiate if there is a sufficient mechanical load. Welded components, such as the stainless steel flasks that store intermediate nuclear waste, may contain significant residual stresses, and additional loads may develop if there is a changes in the dimensions of their contents; hence there is a potential risk of failure. Predicting the likelihood of failure needs data for the time to initiate pits and the criteria for crack initiation.

This project asks the question "Does the criteria for crack initiation depend on whether the pit develops under stress, or if the stress is applied after the pit has developed?" This experimental study will examine the development of pits on salt-contaminated stainless steel under controlled conditions of humidity and

temperature; selected pits will be characterised by high resolution computed tomography. The time to develop cracks will be examined in statically loaded specimens (U-bend) that have been pre-pitted before loading, or have no initial pits. In situ observations, analysed by digital image correlation, may also be performed to examine the kinetics of crack growth. This project does not necessarily require any numerical modelling.

43. Multi-Scale Characterisation of Zirconium-Based Alloys For Fusion Applications

Michael Moody Co-Supervisor(s): Ben Jenkins, Chris Grovenor

Zirconium alloys are commonly used to manufacture the fuel cladding in light water nuclear fission reactors, and many studies have investigated what the optimal processing routes and compositions for these alloys are. However, the higher operating temperatures of fusion reactors render current commercial Zr alloys unsuitable for use, and new alloys need to be designed that display good creep resistance and high temperature strength. Despite this, very little research to date has focussed on the developing Zr-based alloys for nuclear fusion applications.

There is a unique opportunity in the Department of Materials to implement atom probe tomography, a characterisation technique with exceptionally high spatial and chemical resolution, alongside conventional characterisation techniques to characterise a series of novel candidate Zr-alloys for fusion applications. This project will focus on linking alloy composition and processing route with its resulting micro/nanostructure and its macroscale properties.

44. Imaging screw dislocation structures in nanoindented BCC metals

Pete Nellist Co-Supervisor(s): David Armstrong, Jack Haley

BCC metals (including iron, tungsten, chromium and vanadium) are important materials for structural applications in future fusion reactors. Their mechanical properties are largely controlled by their relatively immobile screw dislocations and the formation of sessile locks. The dislocation mobility is thought to relate to the detailed atomic arrangement at the core of the dislocation, but full 3D characterisation of such defects has not before been possible.

This project will perform nanoindentation tests on a range of BCC metals to produce well defined arrays of dislocations. Conventional and recently developed advanced transmission electron microscopy (TEM) methods will be used to investigate the core structure of the dislocations and identify features such as core delocalisation and dissociation The project will make use of mechanical testing, TEM and data analysis in MATLAB and other software packages.

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

Pete Nellist Co-Supervisor(s): 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.

46. In-operando investigation of lithium dendrite formation in liquid electrolyte using dynamic impedance spectroscopy

Mauro Pasta Co-Supervisor(s): Collins Erinmwingbovo

Lithium metal has been reported as the ultimate anode material in unlocking the high specific energy needed for batteries to fully penetrate EV markets due to its low potential (- 3.04 V vs standard hydrogen electrode) and high theoretical capacity (3860 mAh g-1, ca. 10 times that of graphite (372 mAh g-1), which is the currently used anode material in state-of-the-art lithium-ion batteries (LIBs). Furthermore, lithium metal anode is expected to play a central role in emerging battery applications solid-state batteries, lithium-air, and lithium-sulfur batteries. Despite these advantages, the practical application of lithium metal anode has been limited due to several unresolved challenges, one of which is uncontrolled dendritic growth during lithium plating. Lithium dendrite formation has also been reported in lithium/solid-state electrolytes systems.

The mechanism of nucleation and growth of lithium dendrites in organic electrolytes during lithium plating has been theorized to involve uneven current distributions arising from surface inhomogeneities resulting in preferential nucleation in localized hot spots. Several approaches have been reported in the literature to suppress lithium dendrite growth including the use of electrolyte additives, ionic liquid electrolytes, stable lithium hosts, and the utilization of artificial solid electrolyte interfaces. However, the usage of these suppression methods in the lithium metal electrode results often results in increased cost (ionic liquids) and reduced capacity (stable host and electrolyte additives).

Over the years, lithium dendrite formation has been investigated mainly with ex-situ or insitu techniques, which limits our fundamental understanding of the lithium dendrite process in-operando.

In this project, the student will investigate the formation of lithium dendrites in liquid electrolytes using dynamic impedance spectroscopy (DMFA), which allows for direct investigation and observation of processes/phenomena while they are occurring and observe temporal changes in the system.

47. Composite solid electrolytes for Li-metal batteries

Mauro Pasta Co-Supervisor(s): Ed Darnbrough, Georgina Gregory (Chemistry)

The best candidate technology for high energy density batteries for automotive and aeronautic vehicles in the future is all solid state batteries. This new technology has new challenges to traditional batteries and this project will focus on mitigating the volume change during cycling and understanding how to optimise competing factors e.g. ionic conductivity vs active material volume. In this work we will look for you to investigate the interplay between solid electrolyte material, cathode materials and polymer binders to maximise the energy density and effectiveness of an all solid state batteries. This is an exciting space bringing together and building on things you will have learnt about polymers, composite materials and batteries. Within a battery the movement of charges is accompanied with a movement in mass leading to a volume change. In a solid state battery this volume change cannot be accommodated by the liquid electrolyte and more inventive solutions must be sought.

Here is where this project will make an impact looking to suspend active material in a pliable medium that can accommodate the volume change during cycling while without degrading the beneficial electrical properties. This investigation sits within a multidisciplinary collaboration with Chemistry who are developing new polymers for use in this project.

The student will start by considering the role of particle size and active material to polymer ratios on key bulk mechanical and electrical properties. Standard tests will be run in compression and tension to measure mechanical properties and study failure mechanisms while parallel experiments will consider ionic conductivity with polymer thickness. Ultimately this information can be combined to formulate a model for the changes in stress, strain and electrical properties during cycling which can then be probed by running in-operando tests.

48. Chemo-mechanical properties of interfaces in Li-metal based solid state batteries

Mauro Pasta Co-Supervisor(s): Sudarshan Narayanan

As the adoption of electric vehicles increasingly becomes mainstream for both consumers and governments, there is considerable attention being directed towards metrics indicative of performance, efficiency and most importantly, safety, of batteries that form a major component of these vehicles. In this regard, an all-solid-state-approach is fast competing with existing state-of-the-art Li-ion chemistries owing to its potential for improved safety, higher specific energy and power densities. Furthermore, the use of Li metal as an electrode, hitherto infeasible as a result of its poor stability with conventional liquid electrolytes, enables a new class of batteries having much higher capacities. However, Li metal, being very soft and ductile, is prone to deformation via creep during electrochemical cycling, eventually leading to formation of (a) voids at interfaces with solid electrolytes, and (b) dendrites resulting from inhomogeneous plating. As one of the most electropositive metals, Li is also highly reactive and thus readily prone to contamination. Such defects subsequently cause rapid catastrophic failure of electrochemical cells followed by short-circuiting and electrochemo-mechanical degradation.

In this regard, a systematic understanding of the mechanical properties of Li metal and that of its interface with various solid-state electrolytes in determining the electrochemical performance of the cell system is largely lacking. In this project, the student would characterize the topography and mechanical properties of Li metal (and its alloys) surfaces using atomic force microscopy (AFM) and correlate the same with electrochemical cell performance. Following that, the student would conduct a similar study on interfaces of Li metal with well-known solid electrolyte materials (such as sulfides, garnets, antiperovskites, etc.) under “in-operando” conditions using more advanced techniques such as electrochemical-AFM (EC-AFM).

49. Characterisation of ultrafine aerosol particles using single photon detection

Jason Smith

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

50. Compact nutrient sensors for water quality monitoring

Jason Smith

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

51. Magnetic biasing of solid state spin qubits

Jason Smith

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

52. High temperature superconducting thin films for prototype joints

Susie Speller Co-Supervisor(s): Chris Grovenor

The large magnets required for applications in medical MRI and large physics experiments like the LHC at CERN are all based on superconductors and contain numerous joints that are often the (very expensive) points of failure. Understanding the properties of joints between commercial wires and tapes is complicated by their 3D structure and polyphase nature, and this project will fabricate thin films of REBa2Cu3O7 (RE=rare earth) high temperature superconductor and use these ‘ideal’ surfaces to fabricate and test joints to identify the fundamental limits of performance we can then aim for in practical joints between real superconductors.

53. Superconducting bulks for compact NMR/MRI applications

Susie Speller Co-Supervisor(s): Chris Grovenor

MRI and NMR magnets traditionally use bulky and expensive superconducting solenoid magnets. Together with partners at Cambridge University and Oxford Instruments, we are working on cheaper and more compact technologies using high temperature superconductors in the form of bulk pellets that can be turned into permanent magnets. This project will involve analytical microscopy and magnetic characterisation of state-of-the-art materials made in Cambridge to investigate relationships between processing, microstructure and properties.

54. Developing low-resistance interfaces in solid state Li-ion batteries

Rob Weatherup

Solid-state lithium-ion batteries are considered safer alternatives to existing liquid electrolyte batteries, whilst also offering higher energy densities. Existing solid-state electrolytes are typically covered by a surface layer that forms due to reaction with the surrounding atmosphere and leads to increased interfacial resistance, and thus large overpotentials during charge/discharge. Polishing of solid electrolyte pellets is common practice to remove these contamination layers, however this exposes fresh, reactive surface that can quickly form new layers even in an inert glovebox environment. In this project the aim is to investigate whether polishing under certain liquid environments can form an interfacial layer that acts to protect the solid electrolyte from growth of contamination layers as well as facilitating Li-ion conduction. Polished surfaces will be studied by X-ray photoelectron spectroscopy and electrochemical testing (impedance spectroscopy) to track the changes in the interfacial composition as the polishing solution is modified, working towards achieving improved solid electrolyte cell performance.

55. Thin film deposition of battery cathode materials

Rob Weatherup Co-supervisor(s): Susie Speller

Future generations of Li-ion batteries for electric vehicles, require further improvements in energy density which is primarily limited by the cathode (positive electrode) materials currently used. This project will apply pulsed laser deposition to grow thin films of mixed transition metal oxides as high-capacity cathode materials for Li-ion batteries (e.g. Nickel-rich Lithium Nickel Manganese Cobalt Oxides). Different methods to control chemical composition will be investigated, such as deposition from mixed oxide targets and multilayer deposition from multiple targets. These films will be characterised using XRD, SEM and XPS, and the performance of the different materials confirmed through the assembly and electrochemical testing of Li-ion cells (Galvanostatic cycling and impedance spectroscopy). By growing these films on thin (<100 nm) silicon nitride windows, it will then be possible to perform operando X-ray spectroscopy measurements during charging and discharging with XPS and XAS, and to perform post-mortem TEM characterisation of the cycled films.

56. Suspended 2D material membranes for photoelectron spectroscopy of solid-liquid interfaces

Rob Weatherup

PS is one of the most powerful techniques for obtaining surface-sensitive chemical information, by detecting photoelectrons that escape from within a few nm of a surface. However it is typically restricted to solid surfaces under vacuum conditions, limiting its potential applications. This project will involve the development of ultra-thin and impermeable 2D material membranes (Graphene/hexagonal boron nitride) for encapsulating liquids, so that they can be measured using XPS. This will include learning to produce 2D materials by chemical vapour deposition (CVD), and the development of methods to cleanly transfer and suspend them over perforated supports. These suspended membranes will then be characterised optically and with scanning electron microscopy before testing in a vacuum chamber to confirm they are leak-tight. They can then be used for observing liquid-phase catalytic reactions or the accumulation of ions at the graphene interface under electrochemical bias using lab-based XPS systems in the department.

57. Effects of hydrogen on mechanical properties of palladium

Angus Wilkinson Co-Supervisor(s): David Armstrong

The possibility of hydrogen as an energy vector was proposed a considerable time ago but there is a strong resurgence of interest as the need for sustainable carbon free energy systems becomes critical. Palladium could be play a major role in virtually every aspect of a future hydrogen economy, including purification, storage, detection, and fuel cells.

Palladium has the ability to take up large quantities of hydrogen at room temperature and pressure, and subsequently forms palladium hydride (PdHx). This process is reversible and the hydrogen can be subsequently extracted. The effects of hydrogen content, hydride formation and cycling on the mechanical properties of palladium are not well understood.

This project will use nanoindentation, AFM and scanning electron microscopy methods (HR-EBSD and HR-DIC) to study the deformation mechanical properties in virgin and hydrogen charged palladium.

58. Advancing Phase Identification from EBSD Patterns

Angus Wilkinson

Automated analysis of EBSD patterns has led to an incredibly powerful materials characterization method that generates detailed maps of crystal orientation, misorientation, lattice strain and dislocation content. Analysing crystal phases however is limited to distinguishing between best matches of candidate crystals that have already been identified and recorded in a database. A huge drawback is that if a crystal is not in the database then it cannot ever be found. This project aims to implement a very different approach using image analysis methods to search for symmetry elements present in the patterns and from this build up a description of the crystal geometry from first principles. We will develop from ideas described in [1] but using image analysis methods to automate the process, and working towards new functionality within our open source AstroEBSD Matlab code [2].

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

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

59. Dislocation Loops in Irradiated Metals – effects on diffraction peak broadening

Angus 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. 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 likely incorrect [1]. 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 [2].

[1] Balogh et al 2016 J. Appl. Cryst. (2016). 49, 2184-2200

[2] Yu et al 2020, https://arxiv.org/ftp/arxiv/papers/2005/2005.09788.pdf

60. Characterization of Cold Sprayed High Entropy Alloy Coatings

Angus Wilkinson Co-Supervisor(s): David Armstrong,
Tanvir Hussain (University of Nottingham)

Cold spray deposition of metallic coating involves driving powder particles (~10-50 μm) in a high velocity (300-1200 ms^{-1}) gas stream to impact, deform and adhere to the target substrate. In contrast to thermal spraying the metal remains in the solid state which can reduce oxidation issues but implies considerable plastic strain (cold work) is imparted to the particles.

This project will use high resolution EBSD and related advanced SEM based methods to characterise the microstructure and morphology of coatings and substrates generated by collaborators at University of Nottingham [1]. This will be correlated with mechanical properties data obtained by nanoindentation mapping of hardness and modulus. Of particular current interest are high entropy alloy (HEA) CoCrMnNiFe (Cantor alloy) coatings.

[1] http://www.nottingham.ac.uk/CSE

61. 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.

62. 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.

63. Predicting and understanding the colours of molecular crystals.

Jonathan Yates Co-Supervisor(s): Joseph Prentice

Many molecules exhibit the phenomena of polymorphism - the observation that the same molecule can pack together in different ways to form different crystals. This is of major industrial importance, for example pharmaceuticals. Some polymorphs have significantly different optical properties, i.e. their colour. Such molecular crystals have a range of potential applications – inks that can change colour, variable-wavelength lasers, or as a diagnostic tool. The precise conformation of the molecules, as well as the crystal packing, determines the optical properties of the crystal, but a thorough understanding of how is still lacking.

This project would use (time-dependent) density functional theory calculations, running on supercomputers, to investigate how the optical properties of such molecules varies with conformation and crystal packing.

64. Predicting the effect of crystalline environment on the absorption spectrum of molecules

Jonathan Yates Co-Supervisor(s): Joseph Prentice

How strongly a molecule absorbs light at different frequencies is one of its most fundamental properties, and can be of major importance for industrial applications. The absorption spectrum can be strongly affected by the environment of the molecule, including when the molecule is embedded in a crystalline environment. Examples of such systems include hybrid perovskite solar cells, and the recently discovered room temperature maser. However, a thorough investigation of how the crystalline environment could be tuned to achieve the required absorption properties would be very useful.

This project would use (time-dependent) density functional theory calculations, running on supercomputers, to investigate how the optical properties of candidate molecules vary with the crystal environment they are placed within.

65. DFT modelling of rare earth superconductors

Rebecca Nicholls Co-Supervisor(s): Susie Speller

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

66. Predicting the electronic structure of photovoltaic interfaces

Jonathan Yates Co-Supervisor(s): Chris Patrick

A critical step in the operation of solar cells is the separation of electrons from holes to gen- erate an electric current. In the department's Interfaces Lab, next-generation solar cells are being developed which coat the light-absorbing region with nanolayers of other materials to enhance this current generation. How this structure helps the overall device performance will depend on a number of factors, including the electronic structure (band alignment) at the interface. In this computational project we will use density-functional theory (DFT) calculations to investigate these novel solar cell architectures and materials. We will construct models of the surfaces and interfaces and calculate the electronic structure. We will be particularly interested in testing the ability of recently-developed methods in DFT to compute the energy offsets of conduction and valence bands, which traditionally are not well described. There will also be the opportunity to investigate the effects of defects on the electronic structure.

The project will involve a mix of ideas from crystallography, semiconductor materials and quantum mechanics. It would suit a student with good computational skills wanting to apply materials modelling methods to technologically-relevant materials.

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

Jonathan Yates Co-Supervisor(s): Chris Patrick

Some materials with the formula Co2XZ (X = transition metal, Z = main group element) are ex- amples of *half-metallic ferromagnets*. Electrons in these materials show either metallic or insulating behaviour depending on their intrinsic spin, which means that the material's electrical properties (e.g. its resistance) can be controlled with a magnetic field. This effect is exploited in giant magnetore- sistance (GMR) devices. One of the problems with materials like Co2XZ is that their half-metallic properties degrade as the temperature increases. Modelling this effect from first principles is not straightforward, where calculations are most conveniently performed at zero temperature. In this computational project we will use ideas from statistical mechanics and phonon theory to model half- metallic ferromagnets at finite temperature. This will involve some theoretical work building a model, followed by setting up and running density-functional theory calculations.

This project would suit a student interested in using quantum and statistical mechanics to tackle a challenging problem in computational modelling.