DEPARTMENT OF MATERIALS

PART II PROJECTS

2024/2025

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 Wednesday 21st February 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 2024.

Arrangements regarding supervisor availability is given on the next page.

Prospective Supervisors:

Name & Email	Availability
Prof. David Armstrong	Will be in his office on Wed 21 Feb – the 1st floor of 21 BR
Prof. Hazel Assender	Will be in her office on Wed 21 Feb - 4th floor of the ETB, room 40.03
Dr Paul Bagot	Please email to make arrangements to discuss
Prof. Simon Benjamin	Not available on Wed 21 Feb – please email to find an alternative time to discuss
Prof. Harish Bhaskaran	Please email to make arrangements to discuss
Prof. Sebastian Bonilla	Will be in ETB 30.17 on Wed 21 Feb, from 3 to 5 PM
Prof. Peter Bruce	Please email to make arrangements to discuss
Prof. Martin Castell	Please email to make arrangements to discuss
Prof. Marina Galano	Please email to make arrangements to discuss
Prof. Nicole Grobert	Please email to make arrangements to discuss
Prof. Chris Grovenor	Please email to make arrangements to discuss
Dr Rob House	Will be in his office on Wed 21 Feb - the 1st floor of the Rex Richards building, room number 20.42
Prof. Saiful Islam	Will be in his office on Wed 21 Feb from 3 to 4:30 PM – Top floor Rex Richards Building
Dr Anna Kareer	Please email to make arrangements to discuss
Dr Judy Kim	Will be available to discuss online, please email for arrangements
Prof. Angus Kirkland	Available on Zoom from 3:30 PM, please let us know in advance if you want to discuss, to set up a link
Dr Enzo Liotti	Will be in the Holder Café from 3.30pm to 4.30pm on Wed 21 Feb
Prof. Sergio Lozano-Perez	Will be in his office on Wed 21 Feb - the 3rd floor of the Holder building, room number 30.06
Prof. Katharina Marquardt	Please email to make arrangements to discuss
Prof. James Marrow	Will be in his office on Wed 21 Feb from 3 to 5:30 PM - 1st floor of 21BR, room 10.18, can be contacted by email otherwise
Prof. Peter Nellist	Will be in his office on Wed 21 Feb all afternoon – The Holder Tower, Room number 30.05
Prof. Keyna O'Reilly	Please email to make arrangements to discuss
Dr Andrey Poletayev	Will be available on the 3rd floor of the Rex Richards building from 3PM (or via email at any time)
Prof. Rebecca Nicholls	Please email to make arrangements to discuss
Prof. Mauro Pasta	Please email to make arrangements to discuss
Dr Chris Patrick	Not available on Wed 21 Feb, please contact Prof Jonathan Yates or send an email for any project-specific questions
Prof. Jason Smith	Please email to make arrangements to discuss
Prof. Susie Speller	Will be in the Holder Café from 3 PM to 4 PM on Wed 21 Feb
Dr Yige Sun	Will be in the Holder Café from 3 PM on Wed 21 Feb
Prof. Andrew Watt	Please email to make arrangements to discuss
Prof. Rob Weatherup	Will be in his office from 3 PM on Wed 21 Feb - the 1st floor of the Rex Richards building, room 20.09
Prof. Angus Wilkinson	Will be in his office on Wed 21 Feb – 21BR
Prof. Jonathan Yates	Will be in his offce on Wed 21 Feb from 3 PM in Rex Richards

PROJECTS ON OFFER:

1. **Effects of hydrogen on nanomechanical behaviour or materials for a hydrogen energy economy**

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

Zero carbon energy systems are needed urgently and hydrogen has been identified by the UK government as having a key role in future energy systems. However hydrogen is well known to have a deleterious effect on the mechanical properties of many metallic systems. These can include magnesium alloys for hydrogen storage, platinum and palladium in fuel cells, or pearlitic steels in hydrogen transmission. In all cases the effect that hydrogen has on basic mechanical properties is not well understood and an improved understanding will accelerate the development of a hydrogen-based energy economy. Using a new in-situ electrochemical nanoindentation cell this project will compare the mechanical behaviour of industrially important metals with and without hydrogen charging. By working with nano-mechanical testing methods we will be able to correlate the effect of hydrogen on the local microstructural environment around the mechanical test. Combinations of ex-situ and in-situ nano-mechanical testing, will be used along with SEM, HR-EBSD, and AFM characterisation.

2. **Liquid Lithium Corrosion**

David Armstrong Co-Supervisor(s): Chris Grovenor

For nuclear fusion to be a commercial reality, reactors must be self-sufficient in tritium. The likely route for tritium production is through the capture of a fusion neutron by a 6Li atom which produces a tritium atom. Liquid breeding use large volumes of flowing liquid Li or Li-Pb alloys to produce tritium, but has the major disadvantage of the corrosive nature of liquid Li. Currently a range of steels, Zr, W and V alloys have been proposed as structural components, but few corrosion tests have been completed. This project will perform liquid lithium corrosion on alloys of interest to our collaborators in the fusion industry. Alloys could include novel refractories or steels. Samples will be examined using optical and scanning electron microscopy, EBSD and EDX. The aim will be to understand what corrosion products are produced and investigate the effect of different microstructures on corrosion resistance. This understanding will then help inform the engineers designing STEP of the best materials to select.

3. Thermomechanical processing of vanadium alloys

David Armstrong Co-Supervisor(s): Chris Grovenor

Vanadium alloys have been identified as potential candidate materials for structural components in compact nuclear fusion power plant such as the UK STEP device currently under design. This is because they may offer operational temperatures above those of creep resistant ferritic martensitic steels which struggle to operate above 620ºC for long durations.

However, there is a severe lack of data on the vanadium alloy systems being proposed for use in these safety critical applications. Vanadium- chromium-titanium is the most studied system, but In total no more than 150 kgs of material has ever been produced, almost all of it of a very similar composition. There is no consensus on the basic strengthening mechanisms or the optimum microstructure for creep resistance.

This project will develop thermomechanical processing routes for vanadium-based alloys. The V-Cr-Ti system will be used as the starting point with alloys of various composition, cast, mechanically worked and heat treated. Optical, XRD and SEM based methods will be used to study the microstructural evolution, and micro/nano hardness testing to study mechanical properties. If time allows, further strengthening mechanisms such as oxide or silicide dispersions may be explored.

4. A model for radiation-curing of polymers

Hazel Assender

We have used various forms of radiation curing to polymerize diacrylate monomers to a solid, crosslinked polymer layer for coatings in functional materials and devices. Experimental data suggest that the degree of cure depends on the amount of radiation, but also the time it is applied and the depth of material.

This project will seek to model these data and understand the crosslinking behaviour, and subsequent swelling and mechanical properties of the material.

There is scope for practical work to generate more data as required, but the focus of the project will be on the creation of a model to link density of formation of reactive centres (radicals) with the nature of the cross-linked network.

5. Control of diffusion and swelling of hydrogels or elastomers

Hazel Assender

Hydrogels and elastomeric materials find multiple applications in medicine, and control of diffusion and swelling of the material, sometimes over extended periods can be important for applications including drug delivery, tissue engineering and to allow recovery following surgical implantation. This project provides the opportunity for an underpinning study into strategies for control of diffusion and swelling in such materials, including in the increasingly complex shapes that might be applied.

6. Control of long-term drug release for implantable devices

Hazel Assender

Medical implants will often benefit from incorporation of drugs release systems, and there can be a challenge to achieve the slow release of drugs, over long timescales. This project will investigate an approach to achieving very long timescales for drug release in medically implantable materials. This project, has opportunity for collaboration with James FitzGerald, Dept. Surgical Sciences.

The work will involve casting polymer layers, coating deposition and materials characterisation, followed by tracking of large-molecule (drug models) diffusion out of the layers.

There is the possibility to consider improved methodologies for tracking the drug model release.

7. Polymer interlayers for mechanical resilience of thin film coatings

Hazel Assender

Thin film flexible electronic and optoelectronic devices are of substantial technological interest, however in many cases this depends on thin layers of functional, often brittle, materials continuing to perform well even under mechanical bending. We have already shown that introducing a flexible interlayer between the substrate and a relatively brittle functional thin film layer can improve its mechanical resilience.
This project will conduct an underpinning study on a model system (to be decided) that will seek to investigate the parameters that control the efficacy of this interlayer.

8. **Atom Probe Tomography characterisation of critical metals from North Pennine mineral and mine wastes; determining the potential for viable metal recovery**

Paul Bagot Co-Supervisor(s): Luke Daly, Josh Einsle, David Currie (all external)

The transition to a low carbon future relies heavily on an increased usage of metals, many of which can be regarded as energy critical elements. Examples include rare earth elements for permanent magnets used in wind turbines, platinum group elements for catalysis and lithium for battery technologies. Most of these are extracted as by-product or 'companion' metals during mining for other resources. This leads to many of these elements getting left in tailings, slags and other associated mine wastes. Additionally, as extraction technologies evolve the overall composition of waste materials has changed over time, while exposure to weathering conditions will cause these critical metals to mobilise and segregate. Although the overall concentration of such elements is low, they are expected to concentrate as sub-micrometre phases due to the complex, heterogeneous nature of such materials at the nanoscale. In general, both tailings and slags are poorly characterised and understood, yet any critical metals they contain could potentially be economically viable for recovery.

In this project, which is in collaboration with the British Geological Survey (BGS) and the University of Glasgow (UoG), the student will have the opportunity to examine tailings from a mine in the North Pennines. Samples will be down-selected from a variety of legacy waste sites acquired by colleagues, covering a variety of ages. Following on from initial characterisation by Energy Dispersive Spectroscopy and Electron Back Scatter Diffraction in UoG, specific areas of interest will be targeted and specimens for Atom Probe Tomography (APT) will be prepared. APT is a uniquely powerful method to examine the 3D chemical distribution of materials at near-atomic scale. The student will be trained to be a full user in this technique within the Oxford Atom Probe group, characterising the received materials to determine the composition and detailed microstructure of critical elements in the wastes. The project will directly feed into the wider collaboration, giving the student the opportunity to interact with colleagues at partner institutions, and will aim to develop and refine methodologies to use APT to examine and classify such important minerals.

9. Oxidation behaviour of model and ex-service Pt-group alloys

Paul Bagot Co-Supervisor(s): TBC

The industrial production of nitric acid is a critically important part of producing modern fertilisers that support global food production. To produce nitric acid, a key first step is the formation of nitric oxide (NO) by ammonia gas oxidation on heterogeneous catalysts made from Pt-group alloy gauzes. How this oxidation process alters the microstructure of these expensive, often rare metals is poorly understood at present; the outer surface composition can vary markedly from that of the nominal alloy chosen, often a combination of Pt with Rh and Pd.

In this project, the student will use Atom Probe Tomography (APT) to study the atomic-scale microstructures of a range of different Pt-Rh catalyst gauzes and alloys, supplied in collaboration with Yara International, a global Norwegian-based company involved in both developing and utilising these important catalysts. The student will have the opportunity to use a range of supporting characterisation techniques in this work, and have regular meetings with Yara to develop an understanding of applied materials research in an active and important area.

10. 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 2022 a IBM announced a device with over 400 qubits. 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. The concept of quantum error mitigation will likely be key.
    - There are now multiple different kinds of quantum computer prototype that are available online — essentially, research systems similar to those in experimental groups, but usable over the Cloud. It is likely that accessing, exploring and assessing these systems will form part of the main project.

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.

11. Sustainability considerations in nanomanufacturing - a global survey of materials used

Harish Bhaskaran

12. Nanophotonics using functional materials for specific applications - computing, image recognition etc

Harish Bhaskaran

[Please contact Professor Bhaskaran for further details of these projects.]

13. Functional Dielectric Nanolayers in Optoelectronic Devices

Sebastian Bonilla

Field effect devices are used in many applications including computing microchips, memories, and optoelectronic devices. We are particularly interested in the solar energy application of such devices. Many well-known dielectric layers contain permanent charges that can be used to manipulate charge carriers inside semiconductors. We have recently developed a process to tune the intensity of these charges on a silicon substrate.

In this project, the student will first learn and reproduce the processing required to create nanolayers with fixed charge. They will then develop a robust method to design the spatial distribution of the nanoscale dielectric layer as well as the intensity of the charges, which can then be integrated into solar cell precursors.

The student is expected to have a basic understanding of semiconductor devices. The project involves a hands-on fabrication process in a cleanroom environment followed by electrical and optical measurements. The big aim of the group is in accelerating the transition to clean energy by improving solar cell performance while minimising production costs.

14. Laser Processing in Silicon Solar Cell Manufacturing

Sebastian Bonilla

Over the past ten years, the cost of silicon solar panels has rapidly reduced. Solar PV is now the best approach to displace fossil fuel electricity generation and cut CO2 emissions. While current manufacturing of silicon solar cells has advanced rapidly, substantial enhancements in the efficiency and throughput of solar cell manufacturing remain to be made. The exploration and integration of laser-based processes for manufacturing can achieve this. Patterning, structuring and doping via ultra-fine lasers can improve silicon solar cells' performance and longevity. The central objective is to enable the fabrication of improved silicon solar cells by optimising laser patterning and doping processes. This involves investigating the physical mechanisms of the manufacturing processes, understanding how laser beams affect the physical and chemical properties of silicon substrates, and developing optimised protocols for fabrication.

Methodologically, the project will involve using a laser lab-scale facility, and testing various laser processing techniques on silicon substrates. Key activities will include optimising laser parameters such as power, wavelength, and pulse duration, and conducting comprehensive material characterisations before and after laser processing. This will enable performance analysis in processed solar cells under varied conditions. The successful completion of this project could significantly impact the photovoltaic field, offering a new pathway to more efficient and cost-effective solar energy production. This project will require hands-on measurements of the silicon materials in the laboratory and analysis of the generated microscopy, photoconductance and photoluminescence data.

15. Metallisation Technology for Next-Generation Photovoltaics

Sebastian Bonilla

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

This project aims to explore novel contact and metallisation technologies that can address this critical hurdle for the future of solar electricity generation. 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.

16. Semiconductor Device Modelling of Tandem Solar Cells

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. Novel tandem photovoltaic devices have emerged as key enabling technology to achieve improvements in efficiency of solar panels. The main aim of this research project is to develop new finite element simulation techniques with the potential aiding the design and boosting the performance of tandems solar cells, overcoming the drawbacks of conventional single junction solar cells. This project will involve the development of finite element-based computer models to understand and optimise tandem devices. It will use the understanding from other members of the team working on semiconductor processing to test new material concepts and architectures using computer models.

The student is expected to have a strong background and motivation to use computer simulations, and ideally experience with numerical packages like Python, Matlab, or similar. The developments here can impact the development of next-generation silicon-based photovoltaics, and can result in reductions in the cost and wide deployment of solar energy.

17. Challenges in solid-state batteries

Peter Bruce

Conventional Li-ion batteries contain a flammable liquid electrolyte. Replacing the liquid with a solid, enabling the use of a metal anode, will offer higher energy densities and improved safety. However there are a number of challenges that must be tackled and to do this we need to understand the fundamental processes taking place in these cells. All solid state batteries consist of a solid electrolyte, an intercalation cathode, e.g. LiCoO2 or NMC, and an anode with the ultimate goal of this being lithium metal. At the anode, stripping and plating of Li results in void formation and dendrite growth which ultimately lead to cell failure. On the cathode side, expansion and contraction during cycling causes contact loss and rapid capacity fade.

Our research involves developing an understanding of the fundamental science occurring at the material and cell level. This includes investigation of solid electrolyte-electrode interfaces, an important topic in advancing solid-state battery technology. We use this insight to devise strategies to improve performance and extend cycle life.

This project will involve preparing cell components, assembling cells and carrying out electrochemical tests. Alongside this you will use characterisation techniques, such as XRD, SEM and XPS, to understand factors affecting performance.

18. Li ion cathode materials

Peter Bruce

Lithium-ion batteries revolutionised portable electronics and are now playing an important part in an increasing number of technologies, including the electrification of transport. The cathode represents one of the greatest barriers to increasing the energy density and meeting this demand will require new materials.

In current cathode materials, many of which are layered transitional metal oxides, removal of Li during charging is charge compensated by the oxidation of transition metals – limiting energy density. A new class of high voltage cathode materials which store charge on both the transition metals and oxide anions (anionic redox) have the potential to increase energy density by 50%. Several problems have prevented their practical application, including oxygen loss, slow kinetics and structural instability.

Our research explores novel cathode materials for use in Li ion batteries. This involves the synthesis and characterisation of structural, electrochemical and electronic properties to understand the fundamental science underpinning their operation. This project will involve synthesis of cathode materials using methods such as high-temperature solid-state synthesis, co-precipitation and ball milling. You will also assemble coin cells for electrochemical tests and use a number of other characterisation techniques, including XRD.

19. Structural and electronic properties of a metallic monolayer on an oxide crystal surface

Martin Castell Co-Supervisor(s): Chris Patrick

The properties of materials can dramatically change if they are forced to adopt low-dimensional structures. Such structures tend only to be stable in the presence of a second material, as is the case with a monolayer of atoms formed on top of a substrate. In this case, it is possible that the structure of the monolayer, and its associated properties, will be determined by the precise nature of the substrate. This modelling project focuses on Au atoms adsorbed on the perovskite oxide $SrTiO_3$, and will use first-principles calculations to build different potential models of the interface, with a view to finding the most stable structure. The electronic properties will be calculated and compared to the bulk materials. The calculated structures will be used to simulate scanning tunnelling microscopy images to be compared to experimentally measured data. This project would suit a student interested in learning how computational materials modelling can be applied to problems in surface science. As well as computational skills and an interest in electronic structure, strong crystallography skills and an interest in anisotropic thin film strain distributions are also prerequisites for this project.

20. Fabrication of Oxide based ceramic matrix nano-composites for creep applications at 1100°C

Marina Galano Co-Supervisor(s): Talha Pirzada

The proposed Part II project aims to develop the creep resistance properties of existing oxide-oxide ceramic matrix composite (CMC) materials. The project develop nanocomposites by introducing nanoparticles to the developed CMC slurry system to enhance its creep properties, with the aim of producing light-weight, high-temperature, creep-resistant aeroengine components.

The project will include engineering a manufacturing process to produce stable, homogeneous dispersions of nanoparticles in a ceramic slurry. CMC sample panels will be produced using this process and then passed through a test matrix to quantify their mechanical properties. This would include room temperature and high temperature flexural and creep testing, and characterisation of the samples produced (XRT and DVC).

21. Optimising the manufacturing process of Oxide based Ceramic Matrix Composites for heat shields in gas turbine and rocket engines

Marina Galano Co-Supervisor(s): James Marrow, Talha Pirzada

The UK's first prepreg line is being established to produce oxide based prepreg that will be used to manufacture ceramic matrix composite components for gas turbine seals and rocket engine heat shields. Testing needs to be done in order to ensure that the components perform adequately in service conditions.

This project will involve mechanical and morphological characterization of the material system at room and high temperature. This will include room temperature and high temperature flexural and creep testing, and characterization of the samples produced (XRT and DVC). The failure mechanism under load will be identified using 3D strain analysis. Creep tests will be carried out, in tandem with X-ray tomography, on these material systems in order to optimise the layup strategies.
The objectives of this project are:

i. to quantify the mechanical properties of the material system produced in the UK at RT and at 1100°C
ii. to understand the failure mechanisms of these material systems.

22. Synthesis and characterization of plasmonic nanoparticle/TiO_2 fibre hybrid materials

Nicole Grobert Co-Supervisor(s): Barbara Maciejewska

Electrospinning is a well-establish technique using high-voltage to fabricate one-dimensional nano- and microfibres. In conjunction with sol-gel synthesis, it can yield nanostructured ceramics with well-controlled composition and highly modifiable surface properties. TiO_2 fibres that synthesized in our lab have proven to be multi-functional materials manifesting great potentials in biomedical applications, catalysis, water treatments, etc. This project will explore different means to combine plasmonic noble metal nanoparticles with electrospun TiO_2 fibres. A variety of material characterization techniques will be involved to study how the metal-semiconductor interaction can affect the structural, optical, electronic, and chemical properties of the hybrid materials. This project will advance fundamental understanding of plasmonic materials and foster their practical applications.

The project forms an integral part of the research efforts of the group and is aimed at exploring possible application of these hybrid materials, and where possible in collaboration with industry.

23. Fibre reinforced flexible ceramic aerogel for energy, thermal, or structural applications

Nicole Grobert Co-Supervisor(s): Barbara Maciejewska

Ceramic aerogels are a diverse class of highly porous solid materials with many appealing properties such as ultralow density, ultra high thermal stability, and excellent chemical resistance. Yet the conventional ceramic aerogels are extremely brittle and fragile, unable to be practically used. Reinforcing the aerogel structure by ceramic fibres is one of the most popular strategies, in which the fibres enhance the flexibility of aerogel, allow tuning the porous structure, and improve the thermal resistance. This project will exploit using sol-gel synthesis and ambient drying method to fabricate various aerogels, then compositing with the ceramic fibres that have been developed by the Nanomaterials by Design team. The reinforced aerogels will then be characterised, and their properties will be evaluated with view to a series of applications, including gas adsorption, oil/water separation, insulation, etc.
The project forms an integral part of the research efforts of the group and is aimed at exploring possible application of these materials, and where possible in collaboration with industry.

24. Synthesis and characterisation of conductive and elastic carbon nanotube aerogels

Nicole Grobert Co-Supervisor(s): Barbara Maciejewska

Carbon nanotubes (CNTs) are well-known one-dimensional (1D) nanomaterials possessing extraordinary mechanical, electrical, and thermal properties. The key to open up their extensive applications is assembling CNTs into bulk materials while retaining the desired structures and properties. Our lab has been working on CNT-related materials with current professionals in the synthesising of multi-wall and single-wall CNTs using floating catalyst chemical vapour deposition (FCCVD). This project will start with using FCCVD technique to obtain high quality CNTs, then assembling the CNTs into 3D materials (e.g., bulk aerogels) by means of freeze-drying.

The aim of the project is to understand the effect of different parameters to produce aerogels where the CNT are alignment and entanglement well-controlled. The mechanical properties, electrical conductivity and thermal properties will be evaluated and examined. The potential application of such materials will be in the field of thermal management, catalyst scaffold, battery electrodes, etc. The project forms an integral part of the research efforts of the group and is aimed at exploring possible application of these materials, and where possible in collaboration with industry.

25. Tuning the bandgap of TiO_2 nanomaterials towards visible-light driven photocatalysts

Nicole Grobert Co-Supervisor(s): Barbara Maciejewska

Photocatalytic technologies that harvest solar energy are among the hottest research topics in solving the global energy crisis and environmental issues. Titanium dioxide (TiO_2) has been considered as one of the most effective photocatalysts. Downsizing and nanostructuring of TiO_2 lead to a series of superior photocatalysts with strong oxidizing power and exceptional photocatalytic efficiency.

Recently, we developed protocols to synthesize various TiO_2 nanostructures including nanopowders, nanofibres, and mesoporous microfibres. The photocatalytic efficiency of these materials can be boosted by engineering the bandgap. The proposed project will involve synthesising TiO_2 materials using the sol-gel route. Different dopant atoms will be used to tune the electronic structure of TiO_2, therefore manipulating the light absorption especially at visible range. The efficacy of heteroatom doping will be evaluated by photodecomposition of organic dyes.

This project will focus on understanding the light-matter interaction towards designing and developing more effective photocatalysts. The project forms an integral part of the research efforts of the group and is aimed at exploring possible application of these hybrid materials, and where possible in collaboration with industry.

26. Eutectic alloys for solid state battery anodes

Chris Grovenor Co-Supervisor(s): David Armstrong

Storing the highest energy densities in solid state Li batteries requires the use of metallic Li as the anode, but Li metal is very soft, extraordinarily reactive and difficult to use in practical devices. One idea that is being explored to improve the performance is the formation of high Li content alloys. The simple Li-Mg binary system has been studied extensively and has a wide solid solution range, but does not offer the solution to all the practical difficulties. This project will make and test novel eutectic alloys (with Ca, Sr, and or Ba) with the aim of controlling the microstructure/mechanical properties to improve the electrochemical performance. Samples will be examined using optical and scanning electron microscopy, EDX and XRD techniques to establish the as-cast microstructure, to measure the mechanical properties, and the more promising materials will be selected for electrochemical testing in coin cells.

27. Exploring new synthesis routes for oxyfluoride battery cathode materials

Robert House Co-Supervisor(s): Peter Bruce

Increasing the energy density of rechargeable Li-ion and Na-ion batteries is contingent on developing new cathode materials. Recently, disordered rocksalt manganese oxyfluoride cathodes such as Li_2MnO_2F have attracted significant interest as they offer very high energy densities. However, currently they can only be made in nanocrystalline form by ball-milling. This materials synthesis and characterisation project will investigate novel, alternative approaches to access these phases. We will explore methods of fluorinating metal oxides and oxidising metal fluorides and test the products in batteries.

28. Understanding and mimicking mechanochemical synthesis of next generation battery materials

Robert House Co-Supervisor(s): Peter Bruce

Mechanochemical synthesis is a highly effective route for making metastable materials. In the field of battery materials, mechanochemistry has led to the discovery of a whole new class of high energy density cathodes known as disordered rocksalts.

The approach involves milling the reaction precursors together with balls which collide frequently and at high speed. Despite widespread use, the reaction mechanism is very poorly understood. This project aims to ascertain what temperatures and pressures are reached inside the jar, by milling materials which undergo well-known phase transitions. We will then use this information to devise alternative routes to make these metastable materials which mimic these conditions.

29. Mechanical properties of coatings for nuclear fusion

Anna Kareer Co-Supervisor(s): Katharina Marquardt, Angus Wilkinson

For commercially viable nuclear fusion liquid lithium tritium breeder concepts will require a series of coatings to ensure

1) the liquid lithium does not come into contact and react with any underlying metal structure,
2) prevent the diffusion of tritium into underlying materials.

These coatings must be mechanically viable with both good adhesion to underlying material and adequate mechanical properties in their own right. It will also be important to understand how these degrade during service due to thermal cycling and irradiation damage.

In this work a range of transition metal carbides and/or rare earth oxides will be studied using nanoindentation and nanotribology, thermal cycling and SEM based microscopy. The work will be predominantly experimental but analysis will use matlab codes and potentially some finite element modelling.

30. Creation and characterization of defects in graphene for engineering robust graphene liquid cells in transmission electron microscopy

Angus Kirkland Co-Supervisor(s): Adrián Pedrazo-Tardajos, Judy Kim

Nowadays, graphene has multiple applications across various fields due to its unparalleled properties, such as very high electrical conductivity and exceptional mechanical strength. These properties are particularly useful in making graphene an efficient material for supporting a wide range of samples or enclosing different environments in transmission electron microscopy (TEM), thus unlocking in situ TEM experiments to perform studies previously considered unfeasible using the most advanced instrumentation available, such as those involving graphene liquid cells.

However, certain challenges to the obtainment of reproducible graphene liquid cells remain due to the inherent hydrophobicity of conventional graphene.

This project aims to understand and control the correlation between the atomic structure of graphene, with induced defects, and its wettability to yield reproducible, efficient, and robust graphene liquid cells for their implementation in TEM. This work will take place in collaboration with the Rosalind Franklin Institute, enabling access to advanced aberration-corrected electron microscopes equipped with the latest generation of equipment.

The project is ideal for a student with a deep interest in material science, including fabrication and characterization using various techniques. The student will acquire hands-on skills in TEM techniques such as high-resolution imaging and diffraction, necessary for the characterization of dedicated graphene and the preparation of engineered graphene liquid cells, which will have an impact on the fields of TEM and material science.

This laboratory and characterisation work will be undertaken at the Rosalind Franklin Institute on the Harwell Science Campus to utilise the state-of-the-art equipment and work with the staff scientists.

31. Elementally barcoded nanoparticles for biomolecule labelling in electron spectroscopy

Angus Kirkland Co-Supervisor(s): Judy Kim, Brian Caffrey (RFI)

Multielement nanorods have the potential for various applications in the materials and life sciences. However, spatial control of the elemental distribution across the nanorods remain relatively difficult, often leading to heterogeneous nanoparticle mixtures. Recently, Prof. Schaak’s group at Pennsylvania State University has developed a technique to reproducibly control the spatial distribution of elements along copper nanorods. This allows for the generation of thousands of different barcoded labels which can be used as nanometre sized unique identifiers, with potential applications such as intellectual property protection by providing an integrated marker of origin for high value materials or to help determine multiple biological markers of cancer at once, enabling the resolution of protein-protein spatiotemporal relationships.

This project will use synthetic chemical approaches to develop novel elemental combinations of nanorods for elemental imaging using Energy Dispersive X-ray spectroscopy. The aim of this project is to generate elementally barcoded nanoparticles of different shapes and sizes for application in electron microscopy, providing ultra-high spatial resolution over large areas.

32. Investigating the Impact of Recycling on the Mechanical Behavior and Microstructure of Additively Manufactured Materials in Space Applications.

Enzo Liotti Co-Supervisor(s): Yige Sun, Colin Johnston

The project delves into the intersection of sustainable practices and material science within the realm of additive manufacturing. As the utilization of 3D printing and additive manufacturing technologies expands across industries, understanding the repercussions of recycling on the mechanical properties and microstructure of these materials becomes imperative to achieve a more environmentally responsible approach to manufacturing. The research centers around a comprehensive examination of a representative additively manufactured material, employing a controlled printing process to establish a baseline for mechanical properties and microstructure. The subsequent introduction of recyclate material, representing discarded prints and failed components, will subject the components to multiple recycling cycles, simulating real-world scenarios.

The overarching goal is to discern how each recycling iteration influences the material's mechanical behavior and internal structure. The investigation encompasses advanced analytical techniques, including standardized mechanical testing methods and microscopic analyses, to elucidate changes in tensile strength, hardness, impact resistance, and microstructural features. By correlating these findings, the project aims to unravel the nuanced relationship between recycling and the evolving properties of additively manufactured materials. Ultimately, the research outcomes will not only contribute to the academic understanding of material science but also offer practical insights into sustainable manufacturing practices in the growing field of additive manufacturing. This project also extends an invitation to Dr. Alex Goodhand from Satellite Catapult to serve as one of the mentors. This aims to acquaint students not only with academic perspectives from the University but also with industry insights, empowering them for their next career stage.

33. Increase impurity tolerance of recycled aluminium alloys by controlling secondary phase morphology

Enzo Liotti Co-Supervisor(s): Shikang Feng

Aluminium manufacturing is directly responsible for approximately 2% of global CO2 emissions and increasing the recycling rate is urgently needed to accelerate the decarbonization of the sector and meet the 2050 net-zero target. However, aluminium recycling is still a technologically challenging process due to the accumulation of impurities at each cycle, which downgrades the material properties. Impurity elements have the tendency to segregate during solidification and precipitate into harmful intermetallic compounds (IMCs), which can compromise materials performance even at small volume fractions. Removal of these deleterious contaminating elements from end-of-life sources is a huge challenge and the current industry solution to the downcycling problem is to maintain alloy compositions by diluting recycled scrap with virgin, near-pure smelted alloy, with all the attendant logistical, cost and emission penalties. A radical solution is to shift from composition tuning to microstructure tuning, wherein cast components properties are engineered using designed solidification conditions to manipulate impurities into forming benign and finely dispersed second phases, rather than the ’naturally’ occurring detrimental compounds.

Our recent research on secondary phases forming in recycled aluminium with high impurities, which combined in-situ data (X-ray imaging) with electron microscopy post-mortem analysis, showed nucleation of IMCs can be manipulated using ‘inoculant’ and ‘modifiers’ additions (Feng et al., Acta Mat., 221, 117389, 2021 and Feng et al., Mat. Design., 232, 112110, 2023).

Building on this work, this project will investigate the effect of very potent addition on the IMCs formation behaviour in Fe and Si reach commercial alloys. The work will involve the use of high-resolution SEM using EBSD and EDS and possibly in-situ X-ray imaging in the X-ray hutch at Begbroke Science Park. The work will elucidate how to engineer the IMCs in very ‘dirty’ alloys to retained strength and elongation when using low grade scrap materials.

34. Deep Learning for X-ray imaging of metal solidification

Enzo Liotti Co-Supervisor(s): Prof Andrew Zisserman (Oxford Engineering)

X-ray imaging techniques using synchrotron sources have emerged as a powerful tool to study the dynamics of crystal growth, however, the vast and complex data sets generated during multi-modal time-resolved experiments present profound technical and practical problems for quantification. Applying AI to X-ray imaging, including by our group (Liotti et al., Science Advances (2018)), has so far mainly focused on speeding up cumbersome human operations on uni-modal tomographic data, such as volume reconstruction and segmentation, and radiograph post-acquisition analysis. Little work has been carried out on multi-modal deep learning, which therefore remains a difficult challenge as well as an enormous opportunity. The project will focus on the development of algorithms for real-time analysis. Self-supervised vision transformers will be trained for a set of core tasks, such as identification of different solid phases, both in aluminium alloys and steel, and measuring their nucleation and growth rates. These models will then be further trained for more complex tasks to shed light on the interdependency of all the phenomena taking place during metal processing and understand the relationship between the dynamical evolution of microstructure during solidification and the subsequent solid-state transformations.

35. Effect of precipitation on fusion reactor structural materials

Sergio Lozano-Perez Co-Supervisor(s): Jack Haley

Nuclear fusion reactors may require structural materials that can sustain higher-operating temperatures than are currently available to reactor design engineers. Reduced Activation Ferritic Martensitic (RAFM) steels such as Eurofer-97 or F82H typically have an upper limit of 550C, whereas breeder blanket components often have demands for temperatures in excess of 600C. Addressing this disparity between the specification of available materials and design requirements is important to the development of the "DEMO" generation of fusion reactors. UKAEA are therefore developing new RAFM steels, to target these higher-temperature requirements.

These novel alloys being developed require an understanding of how the various precipitate types and sizes are affected by a wide range of heat treatment variables,

such as the normalisation temperature, rolling reduction and temperatures, temper temperature and temper time. However, quantifying a large number of precipitates across a range of scales via conventional SEM-EDX and (S)TEM is slow and difficult. An alternative method is to combine a relatively old TEM-sample preparation method with modern SEM capabilities. The extraction-replica technique is a well-established method for imaging precipitates, without contributions from the matrix material confounding the characterisation. Though recently not a common preparation method, it has been shown to be highly effective for quantifying a large number of precipitates when combined with modern SEM-TKD and EDX. This allows structural phase and chemical information to be mapped quickly and over large areas, allowing for thousands of precipitates to be quantified automatically.

This project is in collaboration with UKAEA (Culham). You will learn to prepare and characterize extraction replicas from novel steels developed for fusion. High-resolution SEM (EDX and/or TKD) will be used to investigate the precipitate structures that have formed over different thermal treatments.

36. High-resolution characterisation of advanced Al alloys for wire arc additive manufacturing of space components

Sergio Lozano-Perez Co-Supervisor(s): Neil Young and Martina Meisnar

Wire arc additive manufacturing (WAAM) is an advanced manufacturing process which has great potential for the production of large-scale spacecraft components such as propellant tank skirtings. Aluminium alloys are great candidates for these components due to their high specific strength, but the best Al alloys need to be adapted to the WAAM process. This project will focus on nano-reinforced Al alloy candidates (2xxx, 6xxx and 7xxx series alloys) that were WAAM manufactured. High-resolution characterisation using SEM (EDX/EBSD) and, potentially, TEM, will be used to investigate the microstructure, texture and defects in the material. A correlation with macroscopic material properties (e.g. mechanical properties, hardness) and comparison with conventionally produced alloys will enable further development of these alloys and the manufacturing process. This project is in collaboration with the European Space Agency (ESA, Harwell).

37. High entropy oxides for humidity sensing

Katharina Marquardt Co-Supervisor(s): Angus Wilkinson

High-entropy ceramics gain increasing attention over the last 20 years due to their ability to combine the favourable properties of their constituent elements. Entropy effects stabilize a simple crystal structure with near equal amounts of 5 or more component elements distributed homogeneously throughout the lattice. These materials have shown increased thermal and environmental stability, interesting electrical and dielectric and catalytic properties. In this study the microstructure of a barium titanate based ceramic with a simple cubic structure that shows unexpected electrical conductivity response in the presence of humidity will be characterized. Skills required, polishing, EBSD and SEM data analysis, Matlab, preferentially also python.

38. SOEC performance in relation to the grain boundary network

Katharina Marquardt Co-Supervisor(s): TBC

Solid Oxide Electrolysis Cells (SOEC) are competitive systems to deliver low-cost, high-efficiency hydrogen production on an industrial scale. A typical SOEC consists of a porous cathode and anode, and commonly a dense electrolyte layer. The porosity enables the transport of fuel and electrolysis products in and out of the cell and increases the reactive surface. The surface crystallography of the particles in contact with pores and the grain boundaries between the particles building the porous structure varies with processing of the SOEC and influences their performance. Yet systematic studies linking electrical performance and degradation to the grain boundary crystallography are not available.

This limits our ability to quantitatively guide material and component design and adjustment of grain boundary structure and crystallography through processing. In this project, we will combine complementing characterization techniques available at Imperial College London and the Department of Materials at the University of Oxford to illuminate the interplay between grain boundary crystallography and the electrical performance of SOEC.

39. Rapid shear deformation - the onset of melting

Katharina Marquardt Co-Supervisor(s): Neil Young, Peter Nellist

In this project the student would do basic TEM diffraction and EDS analysis to understand if the melted material starts to recrystallize.

40. Machine learning for advanced interface recognition and grain boundary energy measurements

Katharina Marquardt Co-Supervisor(s): Angus Wilkinson

In this project the student will work with a large data set of AFM topography maps. Using machine learning they will enable recognition of interfaces and subsequent topography measurements. The tool will enable automated data collection on a wide variety of materials.

41. Tailoring the grain boundary network for enhanced Solid Oxide Electrolysis Cells

Katharina Marquardt Co-Supervisor(s): TBC

Solid Oxide Electrolysis Cells (SOEC) are competitive systems to deliver low-cost, high-efficiency hydrogen production on an industrial scale. A typical SOEC consists of a porous cathode and anode, and commonly a dense electrolyte layer. The porosity enables the transport of fuel and electrolysis products in and out of the cell and increases the reactive surface. The surface crystallography of the particles in contact with pores and the grain boundaries between the particles building the porous structure varies with processing of the SOEC and influences their performance. Yet systematic studies linking electrical performance and degradation to the grain boundary crystallography are not available. This limits our ability to quantitatively guide material and component design and adjustment of grain boundary structure and crystallography through processing.

42. 3D analysis of irradiation creep in nuclear graphite

James Marrow

Irradiation creep is a dimensional change that occurs when graphite is irradiated by fast neutrons whilst under load. It is extremely important for the relaxation of the stresses that develop in the graphite 'bricks' of a reactor core due to neutron dose gradients. Without sufficient creep, these stresses would cause significant cracking of the reactor core components The mechanism of irradiation creep is not well understood, and there are very few data from controlled creep experiments due to the difficulty of these studies. One such experiment was 'ACCENT', conducted by NRG Petten for EDF Energy with support from Frazer-Nash and Atkins. This has provided a unique set of specimens and materials characterisation data for graphite used in the UK AGRs (Advanced Gas-cooled Reactors).

This project aims to answer the question "Does irradiation creep occur uniformly in the graphite microstructure?" The AGR core graphite has a complex microstructure of coarse filler particles in a binder matrix and it is not known if they creep at different rates or not. This is important as there are various graphite microstructures in the UK AGR fleet and their creep behaviour needs to be predicted accurately to support their extended lifetime. New graphites are also being designed and selected for future high temperature gas-cooled reactors, and the potential effects of graphite microstructure on their creep behaviour need to be understood.

ACCENT specimens were imaged by high resolution X-ray tomography (μXCT) both before, and after, their irradiation under load in the High Flux Reactor (Petten). This is a data analysis project, in collaboration with Fraser-Nash, and no experiments will be done. You will apply digital volume correlation (DVC) to the tomographs of selected specimens that developed high creep strains. The aim is to investigate the dimensional change and its degree of anisotropy in the specimens and then to use a local analysis of the data to investigate whether the strains are heterogeneous in the microstructure. DVC can measure the relative three-dimensional displacement field between tomographs, and the analysis that follows on from a recent summer project will follow an approach previously applied to demonstrate differences in the elastic straining of filler and matrix in AGR graphite (http://dx.doi.org/10.1016/j.carbon.2015.09.058j)

43. Analysis of tensile deformation of a ceramic composite by in situ synchrotron X-ray imaging and diffraction

James Marrow

3D needle-punched carbon fibre felts or non-woven cloths are used as the reinforcement in C/C and C/C-SiC composites.

To understand how their damage tolerance is affected by process variables (e.g. thermal stresses) and composite architecture, it is important to observe how damage initiates and propagates (https://doi.org/10.1016/J.COMPSTRUCT.2018.11.041).

This project asks the question "How does the propagation of cracks in the matrix and fibre bundles interact with the process-induced residual stresses?". This is information needed to validate image-based models of composite behaviour (e.g. https://doi.org/10.1111/ffe.12537).

A unique in situ experiment has been performed at the Diamond Light Source (EE17360) to examine the tensile deformation of a 3D needle-stitched C/C-SiC ceramic composite. High resolution synchrotron x-ray computed tomography was combined with diffraction observations to examine the evolution of cracking and stress partitioning between the composite constituents.

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

44. Fracture resistance of thermally oxidised Gen IV graphite

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 measurements of displacement field around the crack tip (http://dx.doi.org/10.1007/s11340-017-0275-1, https://doi.org/10.1016/j.jnucmat.2022.153642), and a recent Part II showed this could be applied to graphite (https://doi.org/10.1520/STP163920210051) This project asks the question “What is the effect of oxidation of the graphite microstructure on the fracture toughness?”.

This experimental study will use optical digital image correlation and digital volume correlation of X-ray computed tomographs to measure, in situ, the displacement fields within a centre-hole notched compression specimens during crack propagation tests. The effects of oxidation on the elastic properties and toughness will be investigated - the effects of thermal oxidation on the graphite microstructure have already been examined. The elastic properties and fracture toughness will be evaluated from these data. The analysis will require some use of finite element modelling methods (Abaqus), and also post-processing of data (Matlab).

45. In situ 3D study of the compressive failure of densified wood

James Marrow

Natural wood is a low-cost and abundant material, but its mechanical performance is unsatisfactory for many advanced engineering structures and applications. Existing pre-treatments (heat/steam etc) can enhance its mechanical properties, but result in incomplete densification and lack dimensional stability, particularly in response to humid environments. Novel processes [https://doi.org/10.1038/nature25476, https://doi.org/10.1016/j.matt.2021.09.020] can now transform natural wood directly into a high-performance structural material with a more than tenfold increase in strength, toughness and ballistic resistance and with greater dimensional stability. The processed wood has a specific strength higher than that of most structural metals and alloys, making it a low-cost, high-performance, lightweight alternative. Proposed applications include a honeycomb core material for battery containment in vehicles.

This project asks the question “How does the heterogeneity of the densification process affect the development of mechanical damage?”. The project, which is in collaboration with Dr Ning Jiang (Shandong University of Technology, China), follows a previous Part II project. You will study the compressive failure of natural and densified wood using in situ high resolution X-ray tomography, analysed by digital volume correlation, to observe the microstructure and mechanisms of damage evolution. The project will involve mechanical testing, computed X-ray tomography and data visualisation (Avizo). It may involve numerical analysis (Matlab), with opportunities to apply finite element simulation with inverse modelling to extract material properties.

46. Controlling damage in electron microscopy characterisation of polymers

Pete Nellist Co-Supervisor(s): Hazel Assender

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

47. 3D strain from 2D images

Pete Nellist

Elastic strain is a hugely important to be able to measure in materials. Strain can control the performance of a wide range of functional materials ranging from catalysts for hydrogen fuel cells to degradation of high capacity Li-ion battery cathodes.

In our group we have developed methods to measure the 2D strain tensor from atomic resolution electron microscope images, where we have assumed that the 2D measured strain is a projection of the full 3D strain tensor. The aim of this project is to model the electron scattering in crystalline materials, which is controlled by the Schrödinger equation, to explore this approximation for a variety of materials. This understanding can then be built on to develop a method to measure the full 3D strain tensor, perhaps using tomographic methods. This computational project will involve electron scattering modelling using existing codes and also developing new methods which can be tested with simulated or experimental data.

48. High speed electron ptychography

Pete Nellist

Electron ptychography is an emerging technique for measuring the phase shift of an electron wave as it is transmitted by a thin sample. Measuring the phase unlocks the ability to detect very low atomic-number elements including Li and O, with a wide range of applications ranging from polymers to Li-ion battery cathodes.
Ptychography makes use of a 4D data set consisting of about a million diffraction patterns recorded using a high-speed camera as an illuminating probe is scanned across the sample. Observations show that the faster the probe can be scanned, the less sample damage will occur, which can be important for samples ranging from polymers to zeolites. By using a specialist detector with only a few pixels, diffraction patterns can be recorded faster than 1 million per second. This is modelling and computational project with use simulations and experimental data to explore the performance of ptychography with few pixel detectors. The project will explore the impact of microscope imperfections and also the extent to which 3D structure can be measured.

49. Oxidation of aluminium alloy melts

Keyna O'Reilly Co-Supervisor(s): Marina Galano

The oxidation of molten aluminium alloys is rather complicated. Several different amorphous and crystalline phases can form. One phase type can transform to another, depending on time, temperature and oxygen levels. Some phases are continuous and protect the underlying melt, others crack and allow mass transport

through the cracks, resulting in run-away oxidation. Some oxide surfaces are smooth, others are covered in nodules. We have determined thermodynamic models which predict which oxide will form for a particular alloy composition and processing conditions. This project will use thermogravimetric analysis (TGA) to monitor the oxidation process and assess the role of kinetics. Oxides will then be extracted from their alloys by a specialist extraction technique and observed using SEM. Data will be used to assess the validity of the thermodynamic models and the role of kinetics.

50. Transport and thermodynamic properties of Na-ion electrolytes

Mauro Pasta

Knowledge of electrolyte transport and thermodynamic properties in rechargeable batteries is vital for their continued development and success. Our group has recently introduced a new method to fully characterize electrolyte systems. [Fawdon et. al. 2021] By measuring the electrolyte concentration gradient over time via operando Raman microspectroscopy, in tandem with potentiostatic electrochemical impedance spectroscopy, the Fickian “apparent” diffusion coefficient, transference number, thermodynamic factor, ionic conductivity and resistance of charge-transfer can be quantified within a single experimental setup.In this project, the student will use operando Raman microspectroscopy to investigate the transport and thermodynamic properties of Na-ion electrolytes and use them to model the performance of Na-ion batteries.

51. Defect engineering in diamond for quantum technology

Jason Smith

The engineering of point defects in diamond promises realisation of memory chips for quantum computing and communications. In Oxford we have pioneered the use of laser processing to create and manipulate defects in controlled ways. The method also opens up a new window through which to observe point defects and their dynamics within diamond and other materials. In this project you will seek to advance our understanding of the processes which occur, the defects created, and the interactions between them. Your focus will be the spectroscopy and analysis of samples produced to study these processes, and you will work within a team of researchers developing the techniques and using them to build devices.

52. Digital chemical sensing in fluids

Jason Smith

Imagine a compact chemical sensor which counts molecules. Worried about toxins in your water supply? Just install a digital chemical sensor and it will alert you whenever a toxin molecule passes through it. We've built devices that do this, but they're currently big and bulky.

In this project you will investigate ways to make them smaller and easier to operate, whilst maintaining their performance. You'll need to enjoy building things in the lab!

53. Development of advanced EBSD techniques for high temperature superconductors

Susie Speller Co-Supervisor(s): Angus Wilkinson

Electron backscatter diffraction (EBSD) is a well-established technique that probes the local crystallography near the surface of bulk materials in a scanning electron microscope (SEM). Diffraction patterns are rapidly collected at each pixel, as the incident electron beam is rastored across the sample. Conventionally, these are indexed automatically using a technique that identifies the positions of the diffraction bands to ascertain the local crystallographic orientation of each pixel. EBSD is a valuable technique for characterising high temperature superconductors, such as REBa2Cu3O7-d (REBCO, where RE=rare earth element) because high angle grain boundaries severely limit superconducting current transport in these materials. However, it is challenging to accurately index REBCO diffraction patterns because the orthorhombic unit cell is very similar to a stack of three cubic cells. This leads to the diffraction patterns for a, b and c-axis aligned grains to be indistinguishable by the standard indexing algorithm.

This project will explore novel pattern analysis techniques, based on template matching to a library of patterns, and/or measuring small shifts in pattern features as is done in HR-EBSD. The Oxford Micromechanics Group has pioneered innovation in EBSD methods.

54. Development of solder-free superconducting joints for MRI magnets

Susie Speller Co-Supervisor(s): Chris Grovenor, Owen Taylor (Siemens)

The magnetic resonance imaging (MRI) medical diagnostic technique uses a low temperature superconducting magnet to produce a highly stable and uniform background magnetic field. To achieve the necessary temporal stability, a closed superconducting circuit - with truly superconducting joints (with a resistance of less than 10-12 ohms) - is required so that the magnet can be operated in “persistent mode” without a power supply. Siemens Healthineers manufacture about a third of the world’s MRI magnets from their factory in Oxfordshire, routinely manufacturing several superconducting joints per day using a reliable lead-based soldering technique. However, under EU regulations, the exemption to use toxic lead in superconducting solders will expire in 2027, and so it is vital that an alternative solution is developed.Since there is no lead-free solder with suitable superconducting performance, this project will involve working with Siemens on a mew solder-free joint method for Nb-Ti multifilamentary wires. The student will have the opportunity to make joints at Siemens and explore the effects of processing conditions on their microstructure and superconducting properties, using analytical SEM and specialist joint testing facilities.

55. Analysis of irradiation damage in atomic resolution STEM images of high temperature superconductors

Susie Speller Co-Supervisor(s): Peter Nellist

High temperature superconductors are an essential enabling technology for compact nuclear fusion power plants. In operation, the highly sensitive superconducting material will be exposed to a high flux of energetic neutrons released by the fusion reaction that create structural defects that degrade superconductivity.
However, very little is known about the nature of the defects that are created, and whether other projectiles (such as light ions that are easier to work with) can replicate the same kind of damage. This project involves developing image analysis and applying simulation techniques to analyse existing high quality atomic resolution scanning transmission electron micrographs on pristine, ion irradiated and neutron irradiated high temperature superconductors, with the aim of quantifying irradiation induced disorder and structural changes.

56. High temperature superconducting thin films

Susie Speller Co-Supervisor(s): Clara Barker

$REBa_2Cu_3O_7$ (REBCO, RE=rare earth element) high temperature superconductor has the capability of carrying large current density in high magnetic fields and at temperatures above the boiling point of liquid helium. This makes them attractive materials for high field fusion magnets.

To achieve high critical current densities in km length flexible tape, REBCO is processed in the form of coated conductor by multilayer deposition on a metal ribbon substrate. Several buffer layers are required in between the metal substrate and the REBCO to avoid chemical reactions, and often impurities are deliberately incorporated to generate defects that improve the current carrying performance. However, the sheer number of elements present in the samples and the complex microstructure makes characterisation of irradiation damage difficult.

In this project, REBCO thin films will be grown directly on single crystal MgO substrates using our pulsed laser deposition facility, to provide much simpler model systems for irradiation damage studies. Film growth will be optimised, by tuning the deposition conditions and using characterisation techniques including x-ray diffraction, scanning electron microscopy, Raman and superconducting property measurements. When a successful recipe has been developed, films will be irradiated with ions at Surrey Ion Beam Centre and re-characterised.

There will be the opportunity for the student on this project to also be involved with synchrotron x-ray absorption experiments on irradiated REBCO.

57. Persistent joints in high temperature superconductors

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 can contain numerous joints that are often the (very expensive) points of failure. Reliable processing strategies are needed to prepare joints between shorter lengths of wire with resistances lower than 10^-12 ohms.

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

58. Superconducting thin films for quantum devices

Susie Speller Co-Supervisor(s): Clara Barker

Qubits and resonators are the building blocks for quantum computers but material challenges significantly limit their potential, with current materials used for convenience rather than by design. This project will carry out fundamental investigations of promising materials for resonators in quantum devices. Thin films will be made using magnetron sputtering, and their material properties tested thorough microstructural characterisation (including XRD, SEM, AFM) and measurement of superconducting properties, using existing and new techniques. These properties will be linked to conditions during film growth, such as power, deposition pressure and temperature. These films will be tested for suitability as quantum resonators, as part of a larger project. This will include converting thin films into resonators (through patterning) and measuring quality factor for the resonators which can also be linked to deposition parameters. The goal of this project will be to study more novel superconducting materials for use in quantum devices, initially Mo:Re but with other materials such as MoN as further options.

59. Nano 3-D Printing

Andrew Watt

The project uses a new solvodynamic printing method developed in Oxford to build three dimensional structures. The project involves:

i. Forming co-solvent based nanowire colloids for printing
ii. Learning to using microfluidic circuits
iii. Programming xyz nano stages to pattern device structures
iv. Testing devices with optoelectronic techniques.

60. Aluminium as an Energy Source

Andrew Watt

Aluminium has one of the highest energy densities of all elements, while at the same time it readily oxidises in to a chemically stable compound. This blue-sky project seeks to utilise aluminium nanoparticles as an energy source.

61. Synthesis of Nanowire Alloys for Photovoltaics

Andrew Watt

Traditionally commercial solar cells rely on silver based inks to form contacts. Silver is inherently expensive, this project seeks to synthesise low cost non-toxic alloy alternates. The project involves:

i. Learning to synthesise nanowires using established methods
ii. Designing synthesis methods for Ag free nanowires (eg CuZnSn)
iii. Forming nanowire thin films and testing their optoelectronic properties.

62. Direct-formation of suspended 2D material membranes

Robert Weatherup Co-Supervisor(s): Jack Swallow

X-ray Photoelectron Spectroscopy is one of the most powerful techniques for obtaining surface-sensitive chemical information, by detecting photoelectrons that escape from within a few nm of a surface. However it is typically restricted to solid surfaces under vacuum conditions, limiting its potential applications. This project will involve the development of ultra-thin and impermeable graphene membranes for encapsulating liquids, so that they can be measured using XPS. This will include using high-resolution 3D printing by two-photon polymerisation to form a perforated support directly onto graphene formed on metal foils by chemical vapour deposition (CVD). The metal will then be etched away to leave the suspended 2D material membrane. These will then be characterised optically and with scanning electron microscopy before testing in a vacuum chamber to confirm they are leak-tight. They can then be used for observing liquid-phase catalytic reactions or the accumulation of ions on the surface of the 2D material under electrochemical bias using a lab-based XPS system in the department.

63. Investigating the role of additives on lithium-ion battery lifetime

Robert Weatherup

Lithium-ion batteries are already widely deployed in portable electronics and increasingly in electric vehicles. To maximize the energy that can be stored it is desirable increase the voltage to which they can be charged, however the LiNi0.8Mn0.1Co0.1O2(NMC) materials commonly used as cathodes are not very stable at high potentials. In order to prolong battery lifetime approaches are needed to stabilise NMC surfaces at high potentials.

In this project we will study different electrolyte additives to suppress unwanted side reactions causing battery degradation. Electrochemical measurements will be performed to evaluate how effective these different additives are in stabilizing the NMC surface, and this will be followed by characterization with various techniques determine how the additives interact with the NMC electrode. This is likely to include x-ray photoelectron spectroscopy (XPS), x-ray absorption spectroscopy (XAS), Differential electrochemical mass spectrometry (DEMS) and electrochemical impedance spectroscopy, but there will be scope to explore other methods as the project progresses.

64. Size-selected multi-component alloy nanoparticles for electrochemical fuel production

Robert Weatherup Co-Supervisor(s): Longxiang Liu

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

This project will use a newly installed deposition source, that forms nanoparticles of controlled size by expanding a metal vapour through a nozzle, and then mass filters these to select only particles of a desired size.

The formation of high entropy alloy particles (containing >5 elements in roughly equal proportions) will be studied and then their sizes and variation in composition characterised using electron microscopy, and X-ray photoelectron spectroscopy. The performance of optimised catalysts will then be investigated for electrochemical water splitting.

65. Water in Salt Electrolytes with Polymer Additives for Li-ion Batteries

Robert Weatherup

Commercial Li-ion Batteries (LIBs) typically use LiPF6 salt in a mixture of organic solvents, which present numerous hazards due to the flammability of the organic solvents and reactivity of LiPF6 with trace amounts of water to form dangerous side products. Water-in-salt electrolytes are a promising alternative for lithium-ion batteries. Unfortunately, the electrochemical stability of WiSEs have not yet been sufficiently improved to be usable in commercial LIBs.

This project aims to achieve reversible cycling with WiSEs by testing new, safer salts in water and combining them with water soluble polymers to form a more hydrophobic passivating layer on the battery electrodes and prevent electrolyte breakdown. This will involve mixing new electrolyte formulations, cyclic and linear sweep voltammetry to determine electrochemical stability windows, electrochemical cycling to determine battery performance, X-ray photoelectron spectroscopy to reveal the composition of the passivating layers that form and Raman spectroscopy to probe the solvation environments of the new electrolytes. Ultimately, the aim is to improve the viability of WiSEs for use in commercial LIBs.

66. Rocket Science - multi-material additive manufacturing for propulsion systems

Angus Wilkinson Co-Supervisor(s): David Armstrong, Martina Meisnar (ESA)

The thrust chambers for ESA’s Ariane 6 launch system involve complex assembly of liner and jacket parts. Multi-material additive manufacture (MMAM) in which different materials are incorporated in a single build with properties tailored to locations. This has the potential to greatly simplify the production, and generate efficiency gains, in this and other space applications.

This collaboration with ESA aims to characterise MMAM microstructures and mechanical properties on the micro-scale. Graded transitions as well as bonding on interfaces will be investigated in materials such as In718/In625, Cu alloys or NiCrAlY. The aim is to understand the properties on the microscale in order to steer the process parameters and processing conditions in the AM process.

67. Scratching the surface: fundamentals of wear

Angus Wilkinson Co-Supervisor(s): Anna Kareer

Wear of materials is a complex phenomenon that is not fully understood despite its presence as a failure mode in many industrial sectors. The development of instrumented indentation systems (nanoindenters) has provided a platform with which the contact of single asperities can be isolated and studied in well-controlled experiments. However, nanoindentation studies use a hard diamond indenter tip to probe a softer flat polished sample surface.

This project will explore a step change by enabling study of metal–metal contacts where more similar mechanical and chemical behaviour may significantly alter the nano-scratch process. The key focus to unlock these import measurements is designing and producing metallic tips reliably. We will explore, coating an existing diamond tip, electrolytic polishing of wires, FIB/pFIB and laser micromachining. Indentation and scratch test will the examine how the tip shape evolves, the tip material work-hardens, any adhesion between tip and substrate, and any material transfer that takes place.

68. High Throughput Testing of Recyclable Sustainable High Entropy Alloys

Angus Wilkinson Co-Supervisor(s): David Armstrong, Desmond Klenam (Witts)

High entropy alloys containing elements that might be readily sourced from waste streams and may provide a sustainable, recyclable utility material – cheap, formable and moderate strength. Quick turnaround and small material volumes are helpful in early stage of alloy design/development. The simple shape and small size possible for bend tests makes them attractive for mechanical properties assessment in these circumstances. However, extracting stress-strain response is not so straight forward, as strain and strain rate varies spatially through the beam.

This project will explore using machine learning surrogate models to extract stress-strain curves from DIC maps of strain evolution during bend tests. Finite element simulations will produce training data sets linked to the known stress-strain response. Then the fast surrogate model will be used for the inverse problem obtaining stress-strain from the experimental bend test data.

Students who are interested in DFT modelling in areas not covered by the listed projects should contact Professor Jonathan Yates for an informal discussion.

69. Machine learning interatomic potentials for battery electrolytes

Zachary Goodwin Co-Supervisor(s): Saiful Islam

We aim to train machine learning (ML) interatomic potentials (IPs) to simulate battery electrolytes, such as conventional Li-ion carbonate electrolytes, with unprecedented accuracy. The work will involve collecting training data for the ML IP from density functional theory, either using classical force fields or active learning to sample uncorrelated structures, which will be used to train an equivariant graph neural network ML IP. We aim to test the bulk solvation structure of the electrolyte from this ML IP, and test the chemical transferability and stability of the ML IP.

70. Transport properties of high entropy liquid electrolytes

Zachary Goodwin Co-Supervisor(s): Saiful Islam

The concept of high entropy materials has recently been demonstrated in the space of liquid electrolytes as a method to improve transport properties. How exactly more components, e.g., the number of different solvents, improve the transport properties of the active ions has not yet been understood, however. We aim to perform atomistic molecular dynamics simulations to compute the transport properties of high entropy electrolytes to understand the origin of this effect. This could also include the development of a machine learning interatomic potential to ensure the predictions being made by the classical force field are qualitatively correct.

71. Sampling surface reactivity of lithium-ion battery cathodes

Saiful Islam Co-Supervisor(s): Andrey Poletayev

The performance of lithium-ion battery cathodes is often limited by the voltage at which they decompose the battery's solvent and evolve gas. This decomposition is a complex surface phenomenon that is challenging to observe experimentally or sample computationally.

Here we will use state-of-the-art machine learning methods to simulate the behavior of industrially relevant nickel-based cathode surfaces in contact with the battery solvents. We expect to focus in particular on the formation of CO2 and O2 gases and understand the mechanisms of these two reactions. The computational results from this project will inform experimental investigations. A familiarity with python, scientific computing more broadly, or basic machine learning will be helpful, while prior knowledge of density-functional theory is not required.

72. Simulation of lithium stripping and plating in a solid-state battery

Saiful Islam Co-Supervisor(s): Andrey Poletayev

The interface between a solid-state ion conductor and the anode, typically lithium metal, determines the stability of the overall battery: the battery can only function if the metal can be controllably electro-deposited and stripped away. This project will study lithium stripping and deposition via atomistic simulation with enhanced sampling in an attempt to approximate and inform experimental studies. Familiarity with python or scientific computing more broadly will be helpful.

73. DFT modelling of iron phosphate battery materials

Rebecca Nicholls Co-Supervisor(s): Saiful Islam

Next generation lithium ion batteries are limited by the cathode material and an incomplete understanding of how the material behaves during operation and degradation. Spectroscopic signals generated by both electron and X-ray beams can be used to probe charged or degraded materials.

This project will use first-principles calculations to simulate spectra from a variety of pristine and charged/defective materials to explore the possibility of using spectroscopy as a way of understanding the operation and degradation of battery materials for potential electric vehicle applications

74. Machine learning atomistic simulations to understand defects in rare earth superconductors

Rebecca Nicholls Co-Supervisor(s): Jonathan Yates, Susie Speller

Rare earth superconductors are the material of choice for generating very high magnetic fields in the next generation of nuclear fusion reactors.

The superconductor will be exposed to high energy neutrons so it is important to understand the defect structures that result from this irradiation, and their influence on material properties. Long time scale molecular dynamics will be used to investigate this phenomena. For accuracy these will be generated from DFT calculations using machine learning methods.

75. Modelling semiconductor/oxide interfaces for next generation photovoltaics

Christopher Patrick Co-Supervisor(s): Jonathan Yates

In many functional devices, such as solar cells, interfaces between different materials are essential to the operation of the device. Increasingly, devices are being designed and fabricated to contain interfaces built of materials which are just 1 nm thick. Understanding what is going on at this tiny scale is a significant experimental (and theoretical) challenge.

One example in solar cells is known as the passivating contact architecture, where interfaces are functionalised to separate electrons from holes and produce a current. However, there are issues with this technology, with defects and impurities creating charge traps that inhibit the flow of current. In this modelling project we will focus on the interface formed between crystalline silicon and the oxide semiconductor TiO_2, building on previous work [ACS Omega 8, 20138 (2023)].

In particular, we will try to understand how oxygen vacancies in the TiO2 affect the electronic structure of the entire interface.

This project would suit a student with a strong interest in semiconductor physics and electronic structure, who is interested in applying computational modelling to functional materials.

76. Structural and electronic properties of ligand molecules on Ag surfaces

Christopher Patrick Co-Supervisor(s): Jonathan Yates

Networks of silver (Ag) nanowires can play a key role in new designs of electronic devices, providing electrically-conductive nanostructures. One challenge is to ensure that electrical conduction is achieved between different nanowires that are not in direct contact. One method of improving this conduction is to introduce ligand molecules which stick to the nanowires and provide links between them.

Although such treatments have been shown to improve the conductivity, there remain some unanswered questions about the atomistic structure of these systems.

In this modelling project we will build models of some ligand molecules absorbed on Ag surfaces to try to understand

(a) how the molecules attach to a single nanowire and
(b) how molecules attached to different nanowires interact to form a bridge.

There may also be opportunity to compare vibrational spectra of adsorbed molecules with experimental data, to validate the models.

This project would suit a student interested in learning how computational materials modelling can be applied to problems in surface science and nanomaterials.

As well as computational skills and an interest in electronic structure, strong crystallography skills are also a prerequisite for this project.

77. Understanding the influence of hydrogen on magnetism in rare earth/cobalt compounds

Christopher Patrick Co-Supervisor(s): Jonathan Yates

The materials with the chemical formula RCo_5 (R = Rare Earth) are the earliest examples of rare-earth transition-metal magnets, which are the most commercially successful permanent magnet materials in use today.

It has been known for some time that these materials can be used to store hydrogen. However, it is only recently that experiments have focused on the effect that this stored hydrogen has on magnetic properties.

In this modelling project we will apply state-of-the-art computational techniques to investigate this phenomenon, particularly on how the introduction of hydogen may cause the preferred magnetism direction to flip through 90 degrees. Due to the lightness of the hydrogen atoms it is anticipated that it will be necessary to perform vibrational calculations to quantify the effects of atomic motion on the magnetism. These methods involve a certain degree of statistical analysis and population sampling, and may require the student to generate and manage rather large datasets. As a result, this project requires the student to be interested both in electronic structure theory and also computational aspects, e.g. the use of Python for scripting and data analysis.

78. Studying the structure and excited states of defect complexes in crystals using computational modelling

Joseph Prentice Co-Supervisor(s): Jonathan Yates

Defects in crystalline semiconductors are very important and interesting systems in a variety of applications, including as candidate qubit systems for building quantum computers. However, the interaction between the defects used for these applications (e.g. the nitrogen-vacancy centre in diamond) and other defects that are present in the material (e.g. carbon self-interstitials) is not well-understood. By examining how the presence of these other defects influences the atomic structure and electronic structure of the centres used for applications, we can understand how robust the desirable properties of these systems are against perturbations, and therefore inform fabrication and usage of them. In this project, the student will use computational techniques, including density functional theory and machine learning potentials, to study this problem for relevant centres in semiconductors such as diamond and silicon.

79. Modelling New Materials for Rechargeable Batteries

Jonathan Yates Co-Supervisor(s): Saiful Islam

Materials performance lies at the heart of the development of green energy technologies such as lithium-ion batteries, and computational methods now play a vital role in modelling and predicting the properties of complex materials.

For the rechargeable lithium battery, the positive electrode is one of the major challenges for new electronics and electric vehicles. In addition, there is a growing interest in sodium batteries as the high sodium abundance makes them attractive candidates for low cost grid-storage.

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

Recent Paper on modelling cathodes:

[1] Sharpe R, et al., 'Redox Chemistry and the Role of Trapped Molecular O2 in Li-Rich Disordered Rocksalt Oxyfluoride Cathodes', J. Am. Chem. Soc. 142, 21799–21809 (2020)
[2] Review on modelling cathodes Islam M S and Fisher C A J, 'Lithium and sodium battery cathode materials: computational insights into voltage, diffusion and nanostructural properties', Chem. Soc. Rev., 43, 185-204 (2014) .