DEPARTMENT OF MATERIALS

PART II PROJECTS

2025/6

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 26th 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 2025.

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 26 Feb - 4th floor of the ETB, room 40.03
Dr Paul Bagot	Will be in office in Hume Rothery Building 20:09
Prof. Simon Benjamin	Please email to make arrangements to discuss
Prof. Sebastian Bonilla	Will be in ETB 30.17 on Wed 26 Feb, from 3 to 5 PM
Prof. Peter Bruce	Please email to make arrangements to discuss
Prof. Martin Castell	Will be in ETB 40.24 on Wed 26 Feb from 3-4
Prof. Marina Galano	Please email to make arrangements to discuss
Dr Zachary Goodwin	Please email to make arrangements to discuss
Prof. Nicole Grobert	Please email to make arrangements to discuss
Prof .Rob House	Please email to make arrangements to discuss
Prof. Saiful Islam	Will be in his office on Wed 26 Feb from 3 to 4:30 PM – Top floor Rex Richards Building
Dr Judy Kim	Please email to make arrangements to discuss
Prof. Angus Kirkland	Please email to make arrangements to discuss
Dr Enzo Liotti	Please email to make arrangements to discuss
Prof. Sergio Lozano-Perez	Please email to make arrangements to discuss
Prof. Katharina Marquardt	Please email to make arrangements to discuss
Prof. James Marrow	Will be in his office on Wed 26 Feb from 4:30 to 5:30 PM - 1st floor of 21BR, room 10.18, can be contacted by email otherwise
Prof. Peter Nellist	Please email to make arrangements to discuss
Prof. Keyna O'Reilly	Please email to make arrangements to discuss
Prof. Rebecca Nicholls	Please email to make arrangements to discuss
Prof. Mauro Pasta	Please email to make arrangements to discuss
Prof. Jason Smith	Avaliable after 4pm in office in 12/13 Parks Road
Prof. Hannah Stern	Will be in office on 12/13 Parks Road
Prof. Susie Speller	Please email to make arrangements to discuss
Dr Yige Sun	Will be in the Holder Café from 3 PM on Wed 26 Feb
Prof. Edmund Tarleton	Will be in Office 40.08 in Holder Tower
Prof. Andrew Watt	Please email to make arrangements to discuss
Prof. Rob Weatherup	Will be in his office from 3 PM on Wed 26 Feb - the 1st floor of the Rex Richards building, room 20.09. Jack Swallow will also be avaliable.
Tamsin Whitfield	Will be in office at 20.08 Banbury Road
Prof. Angus Wilkinson	Please email to make arrangements to discuss
Prof. Jonathan Yates	Will be available in my office (top floor of Rex Richards) from 10:30-11:50am on Friday 28th February.

PROJECTS ON OFFER:

1. "Corrosion" of steels by lithium containing ceramics

Prof. David Armstrong Co-Supervisor(s): Dr Pedr Charlesworth

Nuclear fusion will require breeding of tritium. The leading breeder module designs rely on lithium containing ceramics. These breeder modules are designed to operate between 300 and 700oC. Due to the volatile nature of the lithium ceramics it is know that a certain proportion of the lithium cab ne lost during this heating forming lithium vapour. Recent work in our group has seen that this lithium vapour can condense on steels, react with the steel and cause degradation. This project will use lithium ceramics produced in Oxford or by collaborators and conduct systemic studies to understand the reactions between the steel, ceramics and lithium vapour. The student will learn how to prepare and handle air sensitive samples in a glove box, and use SEM, AFM and EDX to conduct microstructural characterisation.

2. Investigating the impact of recycling on the mechanical behavior and microstructure of additively manufactured polymer materials in space application

Prof. Hazel Assender Co-Supervisor(s): Dr Yige Sun, Dr 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,

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

Prof. 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 Prof 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.

4. Control of diffusion and swelling of hydrogels or elastomers

Prof. 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.

5. Polymer interlayers for mechanical resilience of thin film coatings

Prof. 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.

6. Development of laser ablation sample preparation methods for high resolution characterization

Dr Paul Bagot Co-Supervisor(s) Dr Christina Hofer, Dr Gareth Hughes, Dr Alex Cackett (NNL)

The Atom Probe group in the Department of Materials has recently acquired a femtosecond laser tool (3D MicroMac), capable of cutting and machining materials samples for analysis using advanced techniques such as Atom Probe Tomography and Transmission Electron Microscopy. This approach has the potential to significantly speed up production time of specimens for these techniques, which have often time-consuming current methods using Focused Ion Beams. However, the precise details of how best to use this new method are not well understood; in this project the student will have the opportunity to carry out systematic studies of how to use this laser to prepare samples from a wide range of materials, including steels, nickel alloys, aluminium, zirconium alloys and selected non-metallics. Preliminary studies with this tool have been conducted in collaboration with the National Nuclear Laboratory; Dr. Alex Cackett from NNL will also be co-supervising and advising on material choices. Laser-prepared sections will firstly be examined for the effects of laser damage using electron microscopy methods (SEM, EBSD) within the EM group, while suitably finished APT specimens will later be examined in the atom probe, offering the student the opportunity to become fully proficient in hands-on APT analysis. By the project end, the student should be able to produce a full set of guidelines for use of this advanced laser system on a wide range of materials.

7. Atom Probe Tomography analysis of Aluminium alloys for fission research reactors

Dr Paul Bagot Co-Supervisor(s): Dr Christina Hofer, Dr Andrew London (UKAEA)

Most nuclear fission research reactors (RRs) in Europe are over 60 years old, with only limited infrastructure replacement efforts underway to replace them. Continued safe operation of these reactors is crucial to sustaining European nations’ leadership in nuclear materials and advanced reactor development, as well as ensuring a steady supply of vitally important medical isotopes. Extending the licenses for these reactors requires comprehensive aging reviews and analyses of key structures and components. However, current challenges for this include a limited understanding of irradiation-induced degradation and corrosion mechanisms on RR materials, insufficient surveillance specimens for many reactors, and no standardized approach in Europe for operating RR ageing management. To address these issues, a new project, Research on Materials Ageing and Structural Integrity of Research Reactors (Magic-RR), was launched in November 2024, funded by the EURATOM research and training program, including the University of Oxford and the United Kingdom Atomic Energy Authority (UKAEA). In this project, the student will have the opportunity to be involved in the initial stages of Magic-RR, using Atom Probe Tomography to characterize a range of reference archive Al-alloy materials, then to examine a comparable irradiated alloy as prepared in the active Materials Research Facility at Culham. The student will therefore have an excellent opportunity to engage with a wide network of nuclear researchers both in the UK and within Magic-RR.

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

Prof. 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.

9. Functional Metal Oxide Nanolayers for Tandem Solar Energy Devices

Prof. Sebastian Bonilla Co-Supervisor(s): Dr Theo Hobson

Metal oxide nanolayers, with their unique optical and electronic properties, hold promise for improving light management, charge transport, and stability in next-generation photovoltaics. The project focuses on integrating ultra-thin, optically transparent, and conductive metal oxide layers as interconnects or reflective back contacts within tandem solar cells. The research will involve developing scalable deposition techniques, such as sputtering or atomic layer deposition, to achieve high-quality nanolayers with controlled thickness and uniformity. Advanced characterisation methods, including spectroscopy and electron microscopy, will be used to analyse the optical, electrical, and structural properties of the layers. The ultimate goal is to demonstrate the viability of these nanolayers in tandem device architectures, providing insights into their potential for large-scale deployment in efficient, cost-effective solar technologies. In this project, the student will first learn and reproduce the processing required to create metal oxide nanolayers, then develop a robust method to modify the electronic properties via post-processing methods, which can be integrated into solar cell production. 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 to accelerate the transition to clean energy by improving solar cell performance while minimising production costs.

10. Metallisation Technology for Next-Generation Photovoltaics

Prof. 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.

11. Semiconductor Device Modelling of Perovskite-Silicon Tandem Solar Cells

Prof. 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 investigates how material properties impact the energy yield under varying spectral conditions. Using real-world spectral data measured under diverse weather conditions—from full sun to dense cloud cover—students will analyse performance variations. Experimental data will be complemented by simulations in SunSolve, focusing on tandem architectures. Key objectives include identifying optimal material combinations for maximizing energy yield across dynamic spectra and understanding how spectral variations affect device efficiency. This research bridges the gap between lab-scale performance and real-world applications, providing valuable insights for improving the reliability and efficiency of tandem solar technologies. 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.

12. Lithium-ion cathode materials

Prof. Peter Bruce

Lithium-ion batteries revolutionised portable electronics and are now playing an important part in 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.

13. Challenges in solid-state batteries

Prof. 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.

14. Electrical percolation through a macroscopic random network of conducting and insulating beads

Prof. Martin Castell

Solids consisting of random distributions of conducting and insulating phases are known as electrical percolation materials. They are characterised by a strong non-linear dependence of the electrical conductivity of the whole system versus the relative loading of the different phases. For low conducting element loading there is no conductivity, but as the loading is increased the percolation threshold is reached and limited conductivity is observed. Beyond this point there is a rapid increase in conductivity. Electrical percolation materials are very difficult to manipulate on the microscopic scale because of the random distribution and variability of the shapes of the conducting and insulating phases. For this reason the field is dominated by computational simulations and models using different variations of percolation theory, but there are few systematic experimental studies. In this project small conducting metal and insulating polymer beads are used to create 2D random lattices that form a variety of percolation networks. These experimental observations will be compared with theoretical simulations from a model that is currently under development by a collaborator, Dr Todorov at Queen's University Belfast. The part II student would be expected to optimise the experimental set-up, take extensive conductivity data, and compare this with theory.

15. Fabrication of Oxide based ceramic nanocomposites for high temperature applications

Prof. Marina Galano

"The proposed Part II project aims to develop the creep resistance properties of existing oxide-oxide ceramic matrix composite (CMC) materials. The project will involve 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). The objectives of this project are i) to produce a TRL 3 process for producing stable, homogeneous ceramic slurry containing nano and micro scale particles, and ii) Achieve and verify improvement in creep resistance through nano-engineering of the CMC matrix, microstructure."

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

Prof. Marina Galano Co-Supervisor(s): Prof. James Marrow, Dr 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."

17. Optimisation of SiC/SiC Pre-Preg through Particle Size Variation

Prof. Marina Galano Co-Supervisor(s): Dr Talha Pirzada

"The UK Atomic Energy Authority is developing nuclear fusion capability in the UK, aiming to demonstrate commercial viability and establish a global fusion industry. A critical aspect of this effort is the development of advanced materials capable of withstanding harsh nuclear environments. Silicon carbide fibre-reinforced silicon carbide composites (SiC/SiC) have shown potential for nuclear applications, but improvements in manufacturing methods and material properties are necessary. Recently, UKAEA has developed HASTE-F, a new SiC/SiC material system with a five-fold cost reduction and twice the manufacturability speed compared to conventional chemical vapor infiltration (CVI) methods. This project aims to optimise the HASTE pre-preg material by evaluating the effect of powder particle size on the rheological characteristics of the matrix in slurry form and pre-preg state. Understanding these effects is essential for advancing the manufacturability and performance of SiC/SiC composites for fusion applications.
Objectives • Investigate the impact of powder particle size on the rheological properties of the matrix in slurry and pre-preg forms. • Assess the impact of powder

size on infiltration characteristics and weight loss over time. • Develop an optimised tow-preg material suitable for preliminary lay-up trials"

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

Prof. Nicole Grobert Co-Supervisor(s): Dr 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.

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

Prof. Nicole Grobert Co-Supervisor(s): Dr 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.

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

Prof. Nicole Grobert Co-Supervisor(s): Dr 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.

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

Prof. Nicole Grobert Co-Supervisor(s): Dr 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.

22. Atom probe tomography of Cr-based bcc-superalloys

Dr Christina Hofer Co-Supervisor(s) Dr Paul Bagot, Prof Alexander Knowles (Birmingham)

Cr-based body-centred cubic (bcc) superalloys have emerged as promising candidates for next-generation concentrated solar power applications. These alloys offer several advantages, including a high melting point, cost-effectiveness, and exceptional oxidation resistance, making them well-suited for high-temperature environments. However, optimizing their mechanical properties remains a key challenge in their development. Similar to Ni-based face-centred cubic (fcc) superalloys, coherent, ordered NiAl precipitates can be utilized to enhance strength and creep resistance. In this project, a supersaturated Cr matrix is subjected to various aging treatments to promote precipitation. Previous studies have shown that the addition of Fe increases the solubility of Ni and Al, allowing for precise control over the volume fraction of precipitates and, consequently, enabling the tailoring of the mechanical properties. The student will use scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX) to examine microstructural changes, while atom probe tomography (APT) will provide atomic-scale insights into the precipitation process. The findings from this research will contribute to the design and optimization of Cr-based superalloys for high-performance energy applications.

23. Discovering new ribbon-ordered Na-ion battery cathodes

Prof. Robert House

Oxidation and reduction of oxide ions in layered transition metal oxide cathodes offers a promising route to increase the energy density of rechargeable batteries. Materials possessing a unique ribbon-type ordering of Li and transition metal ions within the transition metal layers, such as Na0.6[Li0.2Mn0.8]O2, are one of the few systems known to support reversible oxygen-redox. This project aims to make new members of this family of compounds based on metals other than Mn. This will enable comparative stability studies to understand how to improve the reversibility of the high voltage oxygen redox reaction.

24. Novel disordered sulfide cathodes for high power Mg-ion batteries

Prof. Robert House

Magnesium-ion is a promising next generation battery technology which does not rely on critical minerals such as Li, Ni or Co. Very recent advances in Mg-ion electrolytes open the door to studies on a much wider range of novel cathode materials. This project seeks to investigate sulfide disordered rocksalts as potential high power cathodes and explore the role of disorder on Mg diffusion in a selection of simple metal disulfide compounds.

25. Quantification of metallic nanoparticles for plasmonic properties using EELS

Prof. Angus Kirkland Co-Supervisor(s) Dr Judy Kim, Dr Adrián Pedrazo (Rosalind Franklin Institute)

In transmission electron microscopy (TEM), TEM grids commonly contain a substrate that supports the sample under investigation, and which is varied depending on the requirements of the sample or experiment. However, the effect of the properties of the substrate, either beneath the sample or acting as an enclosing environment, on the plasmonic properties of metallic nanoparticles has not been thoroughly investigated or fully exploited. Thus, electron energy loss spectroscopy (EELS) will be conducted in state-of-the-art TEM in combination with various substrate materials and environments to quantify the mentioned influence on plasmons. This work will involve learning to use the TEM and EELS at Oxford in order to analyse EEL spectra with the possiblity to contribute to a future publication with the group.

Skills required: basic level of coding, fine motor skills for handling graphene and samples, a meticulous approach for careful microscope operation

26. Image Restoration and Data Processing for Cryo-Electron Ptychography

Prof. Angus Kirkland Co-Supervisor(s) Dr Judy Kim, Dr Amirafshar Moshtaghpour (Rosalind Franklin Institute)

Cryo-Electron Ptychography is a powerful technique for imaging nanoscale details of radiation-sensitive materials like Li batteries, photovoltaics, and biological materials. Ptychography is a computational method applied to Four-Dimensional Scanning Transmission Electron Microscopy (4D-STEM) data. In 4D-STEM, a convergent electron probe scans across a sample and a diffraction pattern is captured at each scan position. This produces a four-dimensional dataset containing both spatial and diffraction information. A key factor in ptychography is the overlapping illumination area, that is the extent to which adjacent scan positions share information. Greater overlap improves reconstruction quality by increasing data redundancy, but excessive overlap results in higher electron fluence, which can damage sensitive samples.

This project will explore the trade-off between scan overlap, image quality, and noise in Cryo-electron ptychography. The student will investigate the sufficient overlap required for accurate reconstructions, assess how noise influences this threshold, identify efficient scanning patterns for a fixed overlap, and evaluate the performance of different ptychography algorithms.

The work will involve large-scale data analysis using Python or MATLAB and will contribute to improved imaging techniques for cryo-electron microscopy. Additionally, this project has the potential for collaboration with Dr. Andrew Maiden at the University of Sheffield.

27. Optimizing beam tilt patterns for electron Fourier ptychography

Prof. Angus Kirkland Co-Supervisor(s) Dr Judy Kim, Dr Jingjing Zhao (Rosalind Franklin Institute)

Ever wondered how we can see the tiniest details of materials and biological structures, and how the details relate to the function? In electron microscopy, phase reconstruction is a beneficial process that helps us reveal fine structural details. One powerful technique for this is Fourier ptychography, a smart computational method that has already enhanced imaging in visible light and X-rays—providing high resolution, a large field of view, and fast acquisitions. When applied to electron microscopy, it has the potential to overcome the conventional axial resolution limits and work with both robust and delicate samples.

As an emerging technique, electron Fourier ptychography has many optimization parameters yet to be explored. This project focuses on identifying the most effective beam tilt pattern—such as a grid or sunflower pattern—for efficient phase reconstruction under different electron dose constraints and target resolutions. Additionally, we will investigate how the overlap ratio evolves with changes in beam tilt magnitude. This research will contribute to the practical application of electron Fourier ptychography in future experiments.

This work will provide students with an opportunity to learn about electron microscopy, phase reconstruction, as well as image simulations. Students are required to have basic skills in programming, such as python or matlab, an understanding of reciprocal space, and a strong foundation in maths.

28. Electron Diffraction for Metal Ion Coordination

Prof. Angus Kirkland Co-Supervisor(s) Dr Judy Kim, Dr Marcus Gallagher-Jones (Rosalind Franklin Institute)

Electron diffraction is a powerful tool for studying ordered materials at the atomic scale. In addition to atomic coordinates, the coulombic potential maps extracted from electron diffraction experiments contain information about charge and bonding potentials. This project seeks to establish the conditions under which it is possible to extract this information accurately. Using energy-filtered 3D-electron diffraction and advanced electron counting detectors, datasets will be captured from well-characterised samples under different conditions. Structures will then be resolved and the voracity of the charge information extracted verified through structure solution and refinement. In addition, some time may be spent simulating diffraction data from different charged species to crosscheck results.

Skills required: Understanding of crystallography, diffraction, familiarity with Python, willing to learn DIALS (https://dials.github.io/about.html) understanding of reciprocal space, and a strong foundation in maths.

29. Defocused Electron Ptychography: Optimizing Parameters of Reconstruction Algorithms for Low-Dose Imaging

Prof. Angus Kirkland Co-Supervisor(s) Dr Judy Kim, Dr Ivan Lobato (Rosalind Franklin Institute)

Electron ptychography has demonstrated significant success in materials science by achieving subatomic resolution—even down to imaging phonon vibrations—and has recently shown potential for biological applications. However, imaging radiation-sensitive specimens presents distinct challenges, including beam induced damage, specimen charging, and sample dynamics. These issues were previously less problematic in materials science, where higher electron doses are typically employed to metallic and ceramics, but has now become an issue to address with current Li-based batteries, zeolite energy storage, and organic-inorganic photovotaics . To mitigate these challenges, imaging must be conducted at lower doses, ideally below 10 $e^{-}/Å^{2}$.

To address this, the project will utilise defocused ptychography, a computational imaging technique in which a convergent electron probe scans a sample while recording a diffraction pattern at each point. This process generates a four-dimensional dataset that captures both spatial and diffraction information. The primary objective is to compare various ptychographic reconstruction algorithms to determine which yields the best results for radiation-sensitive samples, with a particular focus on optimising the algorithms' parameters. As experimental data do not provide a ground truth for these algorithms, the study will rely on simulations from which a ground truth can be reconstructed.

The student will be trained in molecular dynamics simulations to model an atomic-scale system under cryogenic conditions, encompassing a water-buffer environment and rotavirus. Full multislice simulations will subsequently generate convergent beam electron diffraction (CBED) patterns, which will be input into various ptychographic reconstruction algorithms. The initial task involves mastering the different software packages—primarily based on Python (NumPy, TensorFlow, SciPy) and MATLAB—after which the student will evaluate and determine the optimal parameters for each reconstruction method.

30. Increasing recyclability of 7xxx series aluminium alloys for aerospace applications

Dr Enzo Liotti

The 7xxx series is a high value family of aluminium alloys employed mainly in the aerospace sector. However, 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 several approaches to control IMCs formation behaviour in 7xxx series alloys with high level of Fe and Si. 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.

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

Dr Enzo Liotti Co-Supervisor(s): Dr Shikang Feng

Aluminium manufacturing is directly responsible for approximately 2% of global CO_2 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.

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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.

32. High-resolution analysis of sensitisation in 430 stainless steel to improve performance of space hardware

Prof. Sergio Lozano-perez Co-Supervisor(s): Dr Neil Young

AISI 430 Stainless Steel (SS430) is a ferritic stainless steel widely used by industry. In the space sector, it is used for structural parts or valves due to its magnetic properties. The demand for SS430 is high because it offers a favourable balance of cost and performance compared to other alloys. However, at elevated temperatures during service (e.g., heat treatment or welding), SS430 can experience a corrosion damage mechanism known as sensitisation. Sensitisation leads to the precipitation of chromium-rich phases at the grain boundaries, resulting in chromium depletion in the material matrix around it. This phenomenon can cause intergranular corrosion (IGC) and intergranular stress corrosion cracking (IGSCC). It was recently observed that the nitrogen content in SS430 can vary between batches and suppliers ordered for space hardware of the European Space Agency (ESA). As a result, nitrides have been observed at the grain boundaries, similar to carbide precipitation. This effect may be related to the alloy recycling process, where nitrogen is used. This project aims to examine the effect of nitrogen content on corrosion by analysing the formation of chromium nitrides and carbides in alloys exposed to various heat treatments, and how they affect sensitization. Samples will be characterized mostly by SEM, using state-of-the-art EDX and EBSD detectors and, partly, by TEM, to validate SEM findings. This project is in collaboration with the European Space Agency (ESA, Harwell) and frequent visits and interactions with the ESA supervisor are expected.

33. Grain boundary engineering for humidity sensing high entropy ceramics (HEO)

Prof. Tinka Marquardt Co-Supervisor(s): Prof. Peter Nellist

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. The observed fast, reversible change in the capacitance of over 2 orders of magnitude in 800 seconds when humidity was introduced to the atmosphere. It has been speculated an increase in the OH concentration in the crystal lattice or along the grain boundaries causes the increased conductivity. The fast reversibility is yet to be understood but has high potential for industrial humidity sensing applications.

34. Solid Oxide Electrolysis Cells performance related to grain boundary crystallography.

Prof. Tinka Marquardt Co-Supervisor(s): Prof. Angus Wilkinson

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 (Fig. 1) 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).

35. Preventing catastrophic failure: Tuning the grain boundary engineering for W-based fusion shielding materials

Prof. Tinka Marquardt Co-Supervisor(s): David Armstrong

In this project we will explore the fundamental mechanisms of grain and inter-phase boundaries as they are critically affecting material properties linked to mechanical strength, corrosion, and diffusion, just to name a few. Introducing the right type of grain boundaries into the microstructure can increase the overall corrosion resistance by orders of magnitude.
The student will have the opportunity to test a variety of differently processed tungsten composites using micromechanics and explore the grain boundary character distribution (GBCD). The main electron microscopy techniques employed will be electron back-scattered diffraction (EBSD) of bulk specimens in an SEM or high-resolution TEM or STEM of isolated grain boundaries and composites with small grain sizes (50-400nm). The resulting microstructural and micromechanical observations will allow us to inform future material choices.

36. Identifying the grain boundary character in ceramics using advanced transmission electron diffraction: A case study on Solid Oxide Electrolysis Cells.

Prof. Tinka Marquardt Co-Supervisor(s): Dr Mohsen Danaie (ePSIC)

Grain and inter-phase boundaries are important defects within the engineering materials microstructure, critically affecting material properties linked to mechanical strength, corrosion and diffusion, just to name a few. Introducing the right type of GB’s into the microstructure can increase overall corrosion resistance by a factor of two or fracture toughness by orders of magnitude. The established routes into grain boundary character distribution (GBCD) determination are either through electron back-scattered diffraction (EBSD) of bulk specimens in an SEM or high-resolution TEM or STEM of isolated grain boundaries. The former technique is limited to grains larger than ~100-200 nm. The latter approach lacks the number of grain boundary observations needed for statistical analysis.

Non-special boundaries are more frequent compared to special GBs, and consequently the non-special GB have a large effect on the materials properties. Yet most HR-TEM studies are focused on special Σ-GB's, which are rarely the dominant type of grain boundaries in ceramics. Importantly these non-special grain boundaries are the ones with the most flexible structures, sensitive to small variations in processing and are consequently engineerable. We aim to enable high resolution structure analysis across the full variability of grain boundaries in misorientation space by using scanning electron nano-beam diffraction (SEND, Fig.1) to collect scanning diffraction data from large areas of the sample. From this we implement automated segmentation and crystal orientation mapping routines, enabling us to obtain structural information across the whole misorientation space and draw a statistically sound picture of the grain boundary character landscape of ceramics.

37. Strengthening fusion reactor walls: engineering the grain boundary network in SiC fibre composites

Prof. Tinka Marquardt Co-Supervisor(s): Dr D Andrews (Uk Atomic Energy Authority)

Silicon carbide fibre composites offer great potential for use in the walls of a fusion reactor owing to their high-temperature properties. The microstructure of these composites consists of woven SiC fibres in a complex matrix of SiC grown around the fibres. Interfaces in these materials critically influence overall material properties, particularly when the interface composition is altered. Sintering aids used during the production of silicon carbide can change the grain boundary chemistry. In this project, the distribution of elements related to sintering aids will be characterised using TEM. The student will use microstructural observations to inform and refine advanced manufacturing through interface engineering.

38. Carbon capture and storage: CO2 sequestration in anorthite-dominated rocks

Prof. Tinka Marquardt Co-Supervisor(s): Prof. S. Incel (Helmholz Center GFZ, Potsdam)

Rising carbon dioxide emissions contribute to global warming, and despite efforts to reduce emissions, carbon capture and storage (CCS) may be required. CCS allows the permanent storage of CO_2 through mineral carbonation. The rate-limiting step in this carbonation reaction is mineral dissolution, influenced by crystallographic surface orientations. Higher-energy surfaces dissolve faster, aiding ion release and carbonation. Understanding grain boundary energy distribution can improve the efficiency of carbon storage.

The project aims to link CO_2 reaction rates with grain boundary types, helping select suitable rock types for sequestration. The student will measure grain boundary distribution using electron backscatter diffraction (EBSD), among other advanced electron microscopy techniques. Furthermore, the minerals' reactivity with CO_2 will be evaluated, validating whether carbon mineralisation occurs at high-energy boundaries and quantifying sequestration rates based on microstructure. The student will have the chance to work in a multi-national, highly collaborative research group in various research fields, from Materials and Earth sciences to climate technologies.

39. Ceramic coatings to empower versatile, clean, carbon reactors.

Prof. Tinka Marquardt Co-Supervisor(s): Prof. A.Gion (Earth Sciences) Dr C.-M. Pang (Carnot Tech)

The Carnot-Tech system uses supercritical fluid to generate pollution free energy from waste carbon. To operate in the supercritical fluid domain and above the Advanced-Ultra-Supercritical region (750^0C+; 35MPa), Carnot-Tech developed a system consisting of specially designed Multi-Purpose Carbon Reactor, Turboexpander and several one-way valves.

High pressure and temperature requirements can only partially be met by the latest superalloy, Haynes 282. However, Supercritical Fluids are highly acidic and therefore very corrosive, to further enhance the lifetime several ceramic coatings are explored. This proposed project tests and characterises the corrosion resistance of these coatings at relevant conditions.

The student has the opportunity to work in a highly collaborative team in materials and earth sciences, learn about corrosion experiment, characterisation with SEM, EBSD and FIB in collaboration with industry.

40. In-situ study of damage evolution in ceramic fibre composites with novel interfaces

Prof. James Marrow

Ceramic composites have applications in aerospace engines, and also potentially in advanced nuclear fission and fusion energy. Their structural integrity must be assured against microstructural damage, which can affect strength, stiffness and hermetic properties (https://doi.org/10.1038/nmat3497). The mechanical characteristics of ceramic fibre composites are particularly sensitive to the properties of the interface between the fibres and the matrix. This project, in collaboration with Imperial College (London), is concerned with direct observation of interface failure and damage propagation in single tows of SiC fibres in a CVD-deposited SiC matrix, and the effect of variations in the composition and thickness of the fibre/matrix interphase. Novel mini-composite specimens have have been designed, and will be studied in this project in situ during tensile testing with high resolution X-ray computed tomography. Digital volume correlation will be applied to map the 3D displacements within the composites. Your main objective will be to develop a data-analysis method (following https://doi.org/10.1007/s11340-019-00557-5) that will enable you to detect and quantify crack development in the microstructure as a function of the applied strain. This will be applied to investigate the effects of the interphase. This project combines hand-on design of experiments and post-processing of digital data.

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

Prof. 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/Python).

42. The Effect of Oxidation on the Fracture Toughness of Graphites for Advanced Nuclear Fission

Prof. James Marrow

There is a need to measure the fracture toughness and resistance to stress concentrating notches in fine grained nuclear graphites that are critical 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 to measure fracture toughness in small specimens has been developed, which evaluates 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). A recent Part II project 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/Python).

43. Dielectric Layers for Quantum Devices

Dr Greg Mazur Co-Supervisor(s): Prof. Sebastian Bonilla

Quantum devices, such as superconducting qubits and quantum sensors, rely on precise control of their electromagnetic environment to achieve high coherence times and reliable performance. Dielectric layers play a critical role in these systems, serving as insulators, substrates, or capacitive elements. However, imperfections in dielectric materials—such as defects, charge traps, and lossy interfaces—can introduce noise and dissipation, limiting device efficiency. This project aims to investigate and optimize the properties of dielectric layers to enhance the performance of quantum devices. By exploring material selection, fabrication techniques, and characterization methods, the study seeks to identify strategies for minimizing dielectric losses and improving yield of semiconductor based quantum devices.

The project will begin with a literature review of dielectric materials commonly used in quantum technologies (e.g., SiO_2, Al_2O_3, and HfO_2) and their known limitations. Experimental work will involve the preparation of dielectric thin films on suitable substrates, using cleanroom facilities to ensure high purity and control. The dilectrics will be grown on Ge/SiGe quantum wells. Characterization techniques such as ellipsometer or capacitance-voltage (C-V) measurements will be employed to analyze film quality, defect density and breakdown voltage. The fabricated layers will then be integrated into simple quantum device structures (e.g.quantum dots), and their performance will be evaluated using low-temperature electrical measurements in a dilution refrigerator. Data analysis will focus on correlating dielectric properties with device performance, potentially supplemented by simulations of electromagnetic behavior.

44. Oxidation of aluminium alloy melts.

Prof. Keyna O'Reilly Co-Supervisor(s): Prof. 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

45. Transport and thermodynamic properties of Zn-ion electrolytes

Prof. Mauro Pasta Co-Supervisor(s): Dr Ben Jagger, Dr Junyi Zhao

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 Zn-ion batteries.

46. Superconducting microwave antennae for high density quantum memory chips

Prof. Jason Smith Co-Supervisor(s): Prof. Susie Speller, Dr Clara Barker

Electronic and nuclear spins in crystalline materials such as diamond are leading candidates for the storage and manipulation of quantum information, offering the prospect of high-density information storage with millions of quantum bits (qubits) on a single chip. However the control of these spins requires the delivery of magnetic fields alternating at MHz – GHz frequencies, generated by current-carrying wires patterned onto the chip surface, and ohmic heating from these wires presents a significant challenge. This project concerns the exploration of superconducting materials that would eliminate such heating. In this project you will fabricate and test simple devices with niobium (T_c = 9.3K) wires, to establish their use for the control of electron spin of nitrogen vacancy (NV) centres in diamond. You will design devices, take part in their fabrication using sputter deposition, characterise their temperature-dependent electrical properties, and test their usage in spin resonance experiments with an NV centre.

47. Thermal locking of microcavities for nanoparticle characterisation

Prof. Jason Smith Co-Supervisor(s): Prof. Angus Wilkinson

Characterisation of nanoparticles in fluids at low concentrations presents significant challenges due to their very weak interaction with light (low scattering cross section). Optical microcavities can be used to amplify signals associated with scattering and, in addition, to 'weigh' particles by measuring their refractive index. In this project you will build and test an apparatus for detecting and characterising single particles as they pass through a microcavity device. To achieve this requires the 'locking' of a cavity mode to an incident laser using a feedback loop combined with temperature control of the device, which will involve aspects of design and materials selection. The goal of the project will be to demonstrate single particle detection! The project falls within an active area of research within the group and makes use of unique instrumentation and expertise that we have developed over the past 10 years. It is also an area of commercial interest, with a new spinout company, Mode Labs Limited, developing instrumentation for water quality analysis. Within the project you will interact closely with other team members and will consider how the work can be translated to realise practical nanoparticle detectors.

48. Structure and chemistry of colour centres in diamond (experiment)

Prof. Jason Smith Co-Supervisor(s): Prof. Jonathan Yates

Colour centre defects in diamond are leading candidates as physical qubits for chip-based quantum information systems but to realise such devices requires engineering materials with regular patterns of single colour centres that have the required properties. A detailed understanding must be developed of how these colour centres form and the ways in which other defects in the surrounding material affect their properties. This involves a combination of experimental work to measure defect properties and atomistic modelling to match the measured properties with theoretical predictions. Two projects are offered on this topic, one of which is purely modelling and the other focused more on experimental work. The projects will focus on the tin-vacancy complex in diamond, which is formed by first implanting tin ions and then annealing, a process which appears to involve the formation of other defect complexes that include carbon self-interstitials, but the details of which are not yet well-understood. Atomistic modelling techniques including Density Functional Theory (DFT), time-dependent DFT and molecular dynamics will be employed alongside optical spectroscopy of single defects to advance understanding of this system. The projects fit into wider efforts within the groups to investigate this topic and so can be adapted to either 'stand-alone' or be carried out collaboratively.

49. Superconducting thin films for quantum devices

Prof. Susannah SpellerCo-Supervisor(s): Dr 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 through 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 patterning thin films into resonators 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.

50. Irradiation damage of high temperature superconducting thin films

Prof. Susannah SpellerCo-Supervisor(s): Dr Jarrod Lewis

REBa2Cu3O7 (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.

51. Superconducting joints for MRI and NMR applications

Prof. Susannah Speller

Medical MRI and NMR spectroscopy require superconducting magnets 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. This project will involve the development of new approaches for fabricating reliable persistent joints which can carry the enormous currents needed for these applications, using methods that are suitable for the factory floor. Optical microscopy, analytical SEM and XRD will be used to characterise the joint microstructure, and superconducting performance will be tested by fabricating test coils and measuring the magnetic field decay in our dedicated cryostat. There will be opportunities to work on a range of different superconducting materials, including Nb-Ti, MgB2 and high temperature superconductors, including the development of joints between dissimilar superconductors. The superconducting materials group collaborate with Siemens Healthineers, Oxford Instruments and Tokamak Energy on joint development projects.

52. Development of MgB_2 superconducting wires

Prof. Susannah Speller

Magnesium diboride is a promising superconductor for MRI and electric aircraft applications owing to its relatively high transition temperature and simplicity of processing. MgB_2 wires are typically manufactured using a powder-in-tube process using a precursor mixture of Mg and B powders. After wire drawing, a heat treatment is used to react the Mg and B in situ to form MgB_2. Typically heat treatments above 700°C are required, so the sheath material has to be carefully selected to avoid unwanted chemical reactions. The aim of this project is to develop methods to lower the heat treatment temperature required for successful fabrication of MgB_2, without compromising the superconducting properties of the material to enable lightweight Al-based sheath materials to be used for electric aircraft applications. The student will fabricate PIT wires, characterise their microstructure using SEM and XRD, and test the superconducting properties.

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

Prof. Susannah Speller Co-Supervisor(s): Prof. 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.

54. Development of atomic defects in 2D materials as optically detected spin qubits

Prof. Hannah Stern Co-Supervisor(s): Prof. Jason Smith

Atomic defects in wide bandgap materials are a source of optically addressable electronic and nuclear spins that can be used for quantum technologies, such as sensing and networking. Recently, we have discovered that hexagonal boron nitride (hBN) hosts optically addressable spin defects that display microsecond spin coherence at room temperature. We are excited about this discovery because it opens avenues to explore this system for applications in various quantum optical technologies. This project will use optically detected magnetic resonance to explore the spin properties of the hBN defects, with the goal of understanding the limitations to the spin coherence and the response of the spin defect to external applied magnetic field. The project is largely experimental and will involve usage of a scanning confocal microscope. The student will work alongside two other PhD students in a dedicated optics laboratory.

55. Characterisation of room-temperature single-photon sources for quantum technology

Prof. Hannah Stern Co-Supervisor(s): Prof. Jason Smith

Single-photon emitting point defects in wide bandgap solids are attractive for quantum optical technologies due to room temperature operation, versatile emission wavelengths, and simple integration possibilities without need for cryogenics or atom traps. However,for a single photon emitter to be useful for quantum information processing, certain performance metrics need to be fulfilled. Quantum key distribution (QKD) demands high single photon purity and optical quantum computing requires the photons to be indistinguishable. This project will characterise the single photon emission of defects in hexagonal boron nitride (hBN). This will include performing quantum optical experiments (such as Hanbury-Brown-Twiss) using a scanning confocal microscope. The student will work alongside two other PhD students in a dedicated optics lab.

56. Fabrication of 2D devices for optical control of atomic spin defects

Prof. Hannah Stern

Hexagonal boron nitride (hBN) hosts atomic scale defects that are of interest for quantum optical technologies. An important engineering step in the development of this system is the integration of the hBN material to 2D devices, for control of the spin and optical properties. In this project, devices will be fabricated via 2D material exfoliation, transfer and processing. The devices will be benchmarked for their performance using our quantum optical setup. The student will work alongside two other PhD students in a dedicated optics lab, as well as some work in a cleanroom empowering them for their next career stage.

57. Crystal plasticity modelling for Fusion Energy

Prof. Edmund Tarleton Co-Supervisor(s): Dr Eralp Demir, Dr Chris Hardie

You will be part of a team modelling materials for fusion. We are interested in how metals deform and break, based on the underlying physics. This requires writing computer code (Abaqus user subroutines for crystal plasticity and cohesive zone modeling), running computer simulations, and comparing predictions with experiments to validate the model. The models we are developing with UKAEA will feed into the design of the new STEP reactor with the aim of making fusion energy a reality. This project is part of a collaboration between UKAEA and Oxford University to develop predictive models to provide engineering relevant material property predictions throughout service. This will provide a degree of confidence to structural integrity assessments in the design phases and critically provide a means of calibration/validation through service by the testing of surveillance samples. You will join a modelling team in Oxford working in close collaboration with UK Atomic Energy Authority (UKAEA). The Abaqus user subroutines written in Fortran in Oxford (https://github.com/TarletonGroup/CrystalPlasticity), will be used to simulate the influence of radiation damage on mechanical behaviour of fusion relevant alloys for the UK's prototype fusion power plant.

58. Synthesis Plasmonic Metal Nanoparticles

Prof. Andrew Watt Co-Supervisor(s): Dr Christiane Norenberg

A systematic study of the influence of growth conditions (temperature, reagents' concentrations) on the size and size distribution of Gold and Silver nanoparticles grown in aqueous solution using citrate. Making Gold and Silver nanoparticles in aqueous solution is a simple, colourful demonstration of how the optical properties of metal nanoparticles depend on their size and shape. It is therefore often used with school students in science outreach events. Whilst the experiments are straightforward, producing immediate colourful visuals, the results crucially depend on a number of experimental factors, which influence the size and shape of the nanoparticles and with that their optical properties. The aim of the project is to develop a simple recipe and set of instructions that produce reproducible results (narrow size distribution & certain NP size) in the above settings. The project will include the characterisation of the synthesised nanoparticles using UV-Vis spectroscopy and DLS.

59. Nano 3-D Printing

Prof. Andrew Watt Co-Supervisor(s): Dr Enzo Liotti

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. Synthesis of Nanowire Alloys for Photovoltaics

Prof. Andrew Watt Co-Supervisor(s): Dr Enzo Liotti

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

61. Mini Cloud Chamber for AI driven Identification of Unknown Radioactive Elements in Sealed Containers

Prof. Andrew Watt Co-Supervisor(s): Dr Enzo Liotti

The current state of the art for determining radioactive elements uses techniques like semiconductor device direct detection, scintillators or mass spectrometry depending on the information sought. In the early days of high energy physics particles were detected using a cloud or a bubble chamber. It allowed the visualization of ionizing radiation and operates by using a supersaturated vapor that condenses into small droplets along the paths of charged particles, revealing their tracks as they move through the chamber and was analyzed by looking at photographic plates and magnetic fields. From this method alpha and beta particles could be directly detected while gamma and cosmic rays could be indirectly detected using secondary interactions. With the advent of artificial intelligence driven video analysis the cloud chamber became a feasible method to determine radioactive material chemistry. Using AI multiple events in a cloud chamber can be tracked and analyzed. The outcome of this project will be a low-cost compact detection system capable of determining materials composition using very weak signals from behind shielding.

62. Investigating nano-scale phase decompositions in novel refractory alloys

Dr Tamsin Whitfield Co-Supervisor(s): Dr Paul Bagot and Dr hristina Hofer

Refractory alloys, based on high melting point elements including W, Ta and Mo, are being considered as novel high temperature structural materials for applications such as the core of fusion power plants and higher efficiency, hotter, gas turbine engines. In order to be used at these extreme temperatures, alloys will need to have sufficient environmental resistance and therefore, refractory metals are often alloyed with Al or Cr to favour the formation of protective oxide layers. Within these systems, dual-phase microstructures on the order of 5-20nm have been observed following quenching. These microstructures are thought occur due to spinodal decomposition within bcc-bcc miscibility gaps such as those between Ta-Zr and W-Cr, which can be followed by an ordering transition if sufficient Al is present. The presence of these dual phase microstructures has implications for the mechanical properties and oxidation behaviour. Segregation of Al or Cr out of the matrix phase is particularly concerning for the environmental resistance of the alloys, as it may limit the capability of the alloy to form a passivating oxide scale. Consequently, it is important to understand how these nanoscale phases initially form on quenching, their compositions and morphologies and how they evolve during subsequent thermal exposures. This project will use atom probe tomography and SEM to characterise the nano-scale features, their composition and morphology. Alloys will be initially studied following quenching from a solution heat treatment, and heat treatments conducted to see how the microstructures and phase compositions would change in service.

63. Microstructural control in multiphase ultra-lightweight alloys

Dr Tamsin Whitfield Co-Supervisor(s): Prof. David Armstrong

The UK government has set a target to transition all new vehicles to electric by 2035. One of the key challenges for electric vehicles is extending their range. Novel high strength light-weight metals could reduce the density of structural components and increase the range of electric vehicles. Increasing proportion of some of the lightest elements, Mg and Li, can reduce the density Al alloys, but may also lead to the formation of brittle intermetallic phases. In order to utilise lower density alloys careful microstructural control will be needed, to ensure that the precipitates that form, their size and distributions result in ductile, strong lightweight alloys. This project will investigate the effects of increased composition of lightweight elements (Mg or Li) on the phases that form exploring how different cooling rates or directional solidification can be used to control the precipitation. The evolution of precipitate morphologies, how metastable phases transition to stable phases and the impact on mechanical properties will then be considered. A systematic series of alloys will be made in our gloveboxes, thermally annealed and the microstructures and phases produced identified (SEM and X-ray diffraction) and analysed. The mechanical properties will be assessed through hardness or nanoindentation testing to determine how they are impacted by microstructural evolution. This study will assess the potential of these novel lightweight alloys, giving insights into how the microstructures can be optimised further.

64. Embrittlement of steels in hydrogen environments – fundamentals of fracture process

Prof. Angus J Wilkinson Co-Supervisor(s): Prof Andy Bushby (Ultima Forma Ltd), and Prof. David EJ Armstrong

Understanding the fundamental mechanisms of embrittlement of steel exposed to hydrogen are critical to being able to model the failure behaviour of steel structures, such as gas pipelines and enable the transition to a zero carbon future. The embrittlement of steel is considered to be governed by diffusible hydrogen migrating to interstitial sites on cleavage planes, thereby lowering the cohesive energy of the steel. The magnitude of the effect also depends on local microstructural features, such as those at welds. Steel samples and industrial context will be provided by Ultima Forma. The concentration of hydrogen required to reduce toughness is <0.1wppm hydrogen. In regions of high stress (lattice strain), the concentration can rise to >1wppm. Fracture toughness then depends on the combination of global concentration of diffusible hydrogen, local stress, and time for hydrogen to diffuse to the high stress region. Conventional fracture toughness tests do not necessarily capture this behaviour, since crack growth proceeds too quickly. There is evidence in the literature of a slow crack growth mechanism, more akin to stress-corrosion cracking, that is governed by the rate of diffusion of hydrogen to the crack tip stress field. This project will design and conduct very slow rate fracture mechanics experiments to reveal this important mechanism. These will need to establish the actual hydrogen concentrations in the material before testing and crack growth rates in near static loading conditions, together with metallurgical assessment of the microstructure. Multi-physics modelling will be used to aid the experimental design and interpretation of results, through calculation of local crack tip stress fields and associated hydrogen concentrations as a function of time.

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

65. Machine learning interatomic potentials for battery electrolytes

Dr Zachary Goodwin Co-Supervisor(s): Prof. Jonathan Yates

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.

66. Transport properties of high entropy liquid electrolytes

Dr Zachary Goodwin Co-Supervisor(s): Prof. Jonathan Yates

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.

67. Exploring phase transitions in 2D materials with machine learning

Dr Zachary Goodwin Co-Supervisor(s): Prof. Jonathan Yates

In metallic transition metal dichalcogenides (TMDs), commensurate charge density waves (CDWs) emerge from electron-phonon coupling, where the electron density is modulated over a larger length scale than the primitive lattice and there is an associated periodic lattice distortion. We aim to utilise machine learning interatomic potentials (ML IPs) to explore the CDW phase transitions in 2D TMDs. The main aim will be to construct a ML IP for a novel example, using density functional theory as the ground truth, and explore the CDW phase as a function of strain/substrate.

68. Atomistic Modelling of New and Emerging Halide Perovskites for Solar Cells

Prof. Saiful Islam Co-Supervisor(s): Dr Vikram

Solar cell technologies play a critical role in helping to mitigate carbon emissions and climate change. Novel metal halide perovskite materials have shown remarkable properties for next-generation solar cell photovoltaics. Based on the prototype halide perovskites MAPbI3 (where MA = methylammonium) and FAPbI3 (FA = formamidinium), the power conversion efficiencies of the solar cells have shown an unprecedented increase from 3% to more than 26% within 15 years. To further improve the performance and stability of perovskite solar cells, deeper insights and understanding of the defect, transport and passivation properties of the materials are crucial.   This research project at Oxford Materials will focus on using advanced materials modelling and machine learning techniques to study topical perovskite materials based on MAPbI3, FAPbI3 and 2D structures. The important objectives will be to gain new atomic-scale insights into ion migration, defect chemistry, molecular passivation and interface properties.

69. EELS modelling of defects in hexagonal boron nitride for quantum application

Prof. Rebecca Nicholls Co-Supervisor(s): Prof. Hannah Stern

Two-dimensional hexagonal boron nitride (hBN) is able to host single-photon emitting point defects. These defects have an optically detected spin signature which shows strong single-photon emission and microscecond spin coherence, even at room temperatures, making hBN a promising material platform for developing scalable quantum devices that operate at ambient conditions. The defects themselves have not been fully characterized and the aim of this project is to investigate the use of electron energy loss spectroscopy as a method of characterization. The project will involve using density functional theory to calculate spectra from a variety of candidate defect structures, some of which could be responsible for the photon emission.

70. DFT investigation of electron energy loss spectroscopy as a way to characterise hydrogen in zirconium alloys

Prof. Rebecca Nicholls Co-Supervisor(s): Dr Calum Cunningham (UK National Nuclear Laboratory)

Zirconium alloy fuel cladding in a nuclear pressurised water reactor slowly corrodes due to the harsh service conditions, creating free hydrogen which can build up in the cladding and lead to delayed hydride cracking (DHC) and hence component failure. Introducing hydrogen getters, such as yttrium, can mitigate DHC and potentially extend the service life of zirconium alloys, but it is very difficult to accurately locate and measure hydrogen to evaluate the effectiveness of different getters. This project, co-supervised by Calum Cunningham from the UK National Nuclear Laboratory, aims to determine whether electron energy loss spectroscopy (EELS) can identify and locate hydrogen in zirconium-based systems of interest by modelling EELS using density functional theory (DFT).

71. Machine learned interatomic potentials to for the study of disorder in Materials.

Prof. Rebecca Nicholls Co-Supervisor(s): Prof. Jonathan Yates

The recent rapid progress in Machine-learned interatomic potentials (MLIPs) has opened up new areas for materials modelling. Simulations can now be carried out on much larger systems, and for significantly longer timescales, but with the accuracy of DFT calculations. This project will use such techniques for the study of defects, such as those caused by radiation damage. The models will be used for the interpretation of experimental measurements previously obtained using (S)TEM.

72. Modelling Cobalt Nanoparticles for Catalytic Production of Sustainable Fuels

Prof. Rebecca Nicholls Co-Supervisor(s): Dr Jack Swallow, Prof. Robert Weatherup

The surfaces of heterogenous catalyst nanoparticles can dramatically restructure with reaction conditions, influencing their performance for important sustainable reactions. This project will employ density functional theory calculations to study adatom formation on Co surfaces, and how this is altered in the presence of reaction gases such as CO and H2. A recently reported theoretical approach [10.1126/science.add0089] will be extended to predict the extent of restructuring, and this will be compared to our recent experimental studies. There will be potential to explore a range of different absorbate molecules to understand differences in how they influence surface energetics.

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

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

Recently developed imaging methods in electron microscopy have reached the level of precision where charge redistribution due to bonding at the atomic scale can be detected which is an exciting new development. These image data can be quantitatively interpreted by comparison with density functional theory calculations. It has been shown that this approach is feasible in very thin crystals. The current question is whether these measurements accurately take into account either the effects of thermal vibrations of atoms or multiple electron scattering in thicker crystals. This modelling project will aim to develop methods to adapt ab-initio calculations using DFT to electron scattering calculations to enable a truly ab-initio calculation of imaging of bonding.

74. Addressing the challenge of long timescales in the modelling of NMR spectra.

Prof. Jonathan Yates

Solid-state NMR is a highly sensitive probe of atomic scale structure and dynamics. Experimental NMR often relies on electronic structure calculations based on DFT to provide the assignment and interpretation of observed spectra. However, many materials problems have remained out of reach due to the computational cost of DFT simulations, a particular example is modelling ionic diffusion (e.g. for electrolytes in solid-state batteries). In this project we will use state-of-the-art machine learning techniques and DFT simulations to interpret experimental NMR experiments.