Harder, better, faster, **stronger**

Dr Saira Naeem and **Professor Fionn Dunne** explain the research and rationale behind HexMat, a multidisciplinary project with the potential to create superior alloys

How would you describe the aim of the HexMat project?

SN&FD: Through scientific, technological, industrial and public engagement, HexMat aims to make the UK the world leader in the understanding and performance of hexagonal alloys used in the aerospace, energy and defence sectors. These high-value alloys exhibit unusual properties and behaviour stemming from strong anisotropy at the crystal level. The project utilises a broad range of advanced characterisation, experimental testing and modelling techniques to develop a deeper understanding of how these alloys deform and fail, identifying key features of their chemistry and microstructure in order to create stiffer, stronger and lighter structures.

Could you discuss your background and how it led to your role as Principal Investigator of HexMat?

FD: My research is in the micromechanics of deformation and failure in polycrystals. Micromechanics enables a rigorous way to relate the forces applied to crystals and their resultant deformation. This means that we can begin to understand and model how crystals work individually and in groups, thereby determining their collective properties and behaviour. A good example is facet fatigue nucleation in titanium (Ti) alloys, through which our approach has yielded a quantitative understanding of the mechanisms for facet cracks to nucleate in aero-engine components. Another example is in ultrasonic waves and their progression through polycrystals of Ti and zirconium (Zr) alloys, potentially allowing 3D textures to be measured using ultrasonics.

A HexMat postdoctoral research associate (PDRA) networking day was held recently at Imperial College London to encourage collaborations between the institutions involved in HexMat. What were the results of this event?

SN: It was an effective way of bringing together PDRAs from Imperial College London, University of Manchester and University of Oxford to develop group cohesion. PDRAs were tasked with various activities and shown equipment and facilities in order to encourage collaboration. The activities included writing and presenting a research proposal, led by the PDRA Support Group. This was designed so that PDRAs within different thematic areas could bring together their ideas, expertise and knowledge of techniques to work on a given problem identified within the HexMat Programme Grant proposal (eg. use of a technique from the Fundamentals Theme in addressing a problem in the Nuclear Performance Theme). We will continue these networking days in the early stages of the HexMat Programme, and the next two meetings will be held at Manchester and Oxford, focusing on technology transfer and research strategies in industry, respectively.

Since translating the establishment of fundamental understanding into industry-ready technology remains a key problem, these industry-focused workshops will address the identification of recent research for industrial uptake, mechanisms of uptake, the details of exemplar problems to which the research could be applied, such as facet nucleation in the aero industry or texture detection in Zr cladding in the nuclear energy sector, and the likely commercial gains.

The HexMat project also partners with the Big Innovation Centre (BIC). What is BIC and what are the advantages of this partnership?

SN&FD: BIC is a joint initiative by The Work Foundation and Lancaster University, which aims to make the UK a global innovation hub, bringing together the world's leading academics, industries and governments. It is an effective platform for key emerging technologies from sectors that would not typically interact, leveraging disparate areas of expertise to inspire creativity and innovative approaches with the aim of making the UK an international leader in innovation, while stimulating economic growth.

The BIC partnership enables us to draw on the best university research to promote innovation and investment, increase our industrial end-users and strengthen advocacy for materials science and engineering. BIC offers proactive engagement with industry leaders and government, ensuring the UK's leading technology in hexagonal metals is represented properly in trade meetings and inspiring new business and investment from overseas.

Beyond its importance for scientific progress, the HexMat project will have important implications for climate change and nuclear energy. Could you explain these in more detail?

SN&FD: Any research that leads to stronger, lighter materials in aerospace and transport applications helps reduce both fuel consumption and pollution. Moreover, the development of alloys for irradiated environments allows the fabrication of components with longer structural integrity and safer operation, making nuclear energy generation more economical.

Advanced alloys

The ambitious **HexMat** project is bringing together a consortium of three UK universities with industrial partners from the aerospace, energy and defence sectors aims to make the UK a world leader in hexagonal alloy systems

ALLOYS SUCH AS titanium (Ti), zirconium (Zr) and magnesium (Mg) have a hexagonal, close-packed (hcp) crystal structure and a wide range of industrial applications. Due to their strength, durability, light weight and resistance to corrosion, UK industry uses them extensively, and they are of profound strategic importance to its economy. Aero-engine manufacturers use these alloys to build components such as blades and discs in engines, while the health industry employs them in the creation of implantable devices such as knee or hip joints. Applications in the energy sector include the creation of components for nuclear power plants, while magnesium alloys have potential applications in vehicle manufacturing. This versatility and resultant ubiquity means that hcp alloys are subject to numerous stresses across a broad range of industrial applications and can become fatigued, leading to undesirable behaviours such as large deformations, shearing or failure, and potentially catastrophic results. Improving the robustness of these materials is therefore a matter of vital importance to UK industry.

STEP-CHANGE

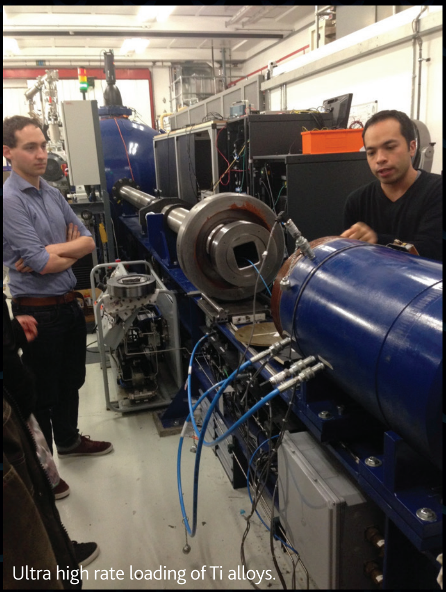
Professor Fionn Dunne is the Principal Investigator for the 'Heterogeneous mechanics in hexagonal alloys across length and time scales' (HexMat) programme. It is a project comprised of teams from three UK universities – Imperial College London (Dunne), University of Manchester (Professor Michael Preuss) and University of Oxford (Professor Angus Wilkinson) – that aims to transform understanding of the fundamental mechanistic processes governing the behaviour of hcp alloys. Through a range of experimental, characterisation and modelling techniques, HexMat is working to generate pioneering technology with the potential to improve radically the performance of existing materials, while exploiting new hexagonals developed virtually using computer tools. "If we can identify the deformation mechanisms controlled by microstructure, morphology and crystallography and incorporate these into computer modelling techniques, it might be possible to create step-change improvements in the performance of a whole range of materials and components across the aerospace, nuclear, energy and transport industries," explains Dunne.

In the hope of improving the durability of these materials, the HexMat team is examining key research topics, including the formation of facet cracks and shear bands, the morphology and crystallographic orientations of the best microstructures, best practices for measuring material textures and how irradiation changes important properties of hcp alloys.

The project outputs are manifold and highly relevant to the academic community, and should be useful to solid-state physicists, metallurgists and multi-scale material modelling research communities, as well as the postdoctoral researchers and graduate students appointed on the HexMat Programme Grant and other members of the research team. "The provision of high-quality trained postgraduates and postdocs is a key impact of our project, and our graduate students and postdocs gain extensive experience in the multi-disciplinarity of industrial pull and research uptake," reveals Dr Saira Naeem, HexMat Project Manager. "The flow of knowledge and skills through to other universities and industries, with close input from our hex-industry workshops and technology transfer programme, enables the project outputs to be exploited by academic and industrial groups alike."

INTERDEPENDENCY

The project has identified four key and interdependent themes. Their first focus is fundamental mechanisms. Through this theme, the group aims to utilise micro- and nano-scale testing to better understand single and oligocrystal properties and behaviour across the range of alloys for both aero and nuclear applications. The second area of interest – micromechanics – applies modelling techniques to Ti, Zr and Mg alloys, building a mechanistic


Ultra high rate loading of Ti alloys.

INTELLIGENCE

HEXMAT

HETEROGENEOUS MECHANICS IN HEXAGONAL ALLOYS ACROSS LENGTH AND TIME SCALES

OBJECTIVES

- To transform understanding of the fundamental mechanistic processes governing the behaviour of hexagonal, close-packed (hcp) alloys through a range of experimental, characterisation and modelling techniques
- To generate pioneering technology with the potential to radically improve the performance of hexagonal alloys in the transport and energy sectors

KEY COLLABORATORS

Professor Michael Preuss, University of Manchester, UK

Professor Angus Wilkinson, University of Oxford, UK

PARTNERS

Rolls-Royce • Westinghouse • EDF Energy • Timet • AMEC

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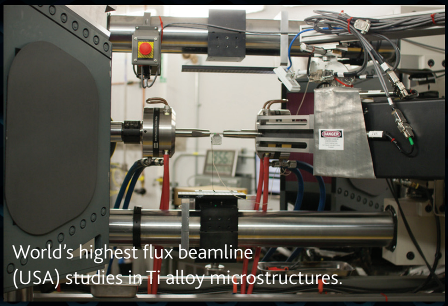
SAIRA NAEEM completed her MSci in Chemistry at University College London, UK, and then worked at the Institute of Cancer Research before joining Imperial College London, UK, as a postgraduate, obtaining her PhD in 2012. She continued her research on transition metal chemistry as a postdoctoral research associate and since July 2013 has worked as HexMat Programme Grant Manager in the Department of Materials.

FIONN DUNNE is Chair in Micromechanics at Imperial College London, UK. He leads the EPSRC Programme Grant HexMat, and directs the Imperial Rolls-Royce Nuclear University Technology Centre. He is Associate Editor of Philosophical Magazine and co-author of Introduction to Computational Plasticity, OUP, 2005. He is Fellow of the Royal Academy of Engineering.

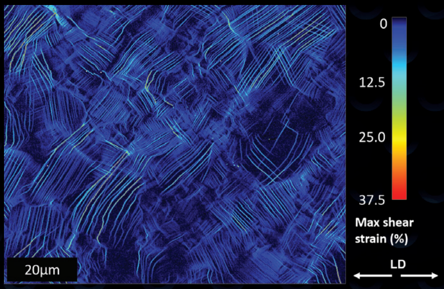
understanding of their properties while addressing 3D texture measurement and defect detection. As a third research topic, HexMat members are examining hcp alloy performance in aerospace environments. These endeavours apply the techniques and knowledge yielded by its predecessors to problems of relevance to the aerospace industry, including why facet fatigue occurs and what the best titanium microstructures are, as well as the chemistry required to form them. Their final research area focuses on pertinent issues in nuclear energy generation, including the problem of pellet-cladding interaction, texture measurement in Zirconium alloys and how irradiation can lead to flow localisation and failure. While performing research into all four of these themes, HexMat employs various modelling methodologies, micromechanical testing, non-destructive evaluation (NDE), characterisation and microscopy techniques.

TIGHT NETWORKING

Close collaboration is vital to HexMat, with each group across the universities bringing something unique to the table. Imperial College London leverages its expertise in microstructural crystal deformation and failure modelling, X-ray diffraction, ultrasonic phased array techniques and very high rate loading tests. These are complemented by the 3D tomographic imaging and powerful transmission electron microscopy (TEM) structure and chemical analysis facilities at University of Manchester, while University of Oxford contributes expertise in micromechanical testing, high resolution electron backscatter diffraction (EBSD) and crystal property extraction.


World's highest flux beamline (USA) studies in Ti alloy microstructures.

The project has also established a consortium of industrial collaborators including AMEC, EDF Energy, Rolls-Royce, Timet and Westinghouse, all of whom are major stakeholders in hexagonal metals. These crucial industrial partners are represented on the project steering board and help to define the key scientific questions for the research, as well as providing valuable knowledge around industry uptake of research, and technology readiness and transfer. The partners also offer support to HexMat's graduate students and postdoctoral researchers, maximising the programme's relevance to industry needs. The HexMat Management Board meets on a monthly basis to discuss the research progress and maintain close links between collaborators; these meetings give the



High resolution digital image of deformation in a Ti alloy.

principal investigators on the four themes an opportunity to discuss tactical management and implementation of risk management decisions, user engagement strategy and impact plans.

Dunne and his colleagues understand that this tight networking constitutes an essential part of the projects. "A key challenge lies in ensuring that we exploit the techniques and expertise available across the collaborating universities and industrial partners as best as we possibly can," he explains. "This is achieved by utilising communication technology, secondments and visits, and we have developed a great team of researchers bound together by the HexMat vision of transforming our understanding of hcp metals."

RAPID GAINS

The project is making substantial progress, with recruitment of postdoctoral researchers across the consortium nearing completion and individual research projects well underway at the three universities. Preliminary results are promising and the team expects to see rapid gains in several areas, including its understanding of cold dwell facet fatigue in explaining the roles of chemistry and microstructure in facet nucleation, potentially leading to the identification of Ti alloy microstructures that inhibit or even prevent such fatigue. They have also completed proof-of-concept work on the ultrasonic measurement of 3D textures, and the next phase of this research will potentially lead to the development of measuring devices with industrial applications. HexMat is also generating novel modelling techniques that will soon allow researchers to quantify and predict the role of irradiation on alloy behaviour, opening up yet more possibilities in the continuing quest for superior component design.