

Future Materials Conference

UNIVERSITY OF BIRMINGHAM

#FUTUREMATERIALS

MIDAS



HENRY ROYCE INSTITUTE

13 DECEMBER 2021



Future Materials Conference

Introduction

Hello and welcome to the 2021 Future Materials Conference!

It is a pleasure to welcome everyone to the first physical event being held by the Student and Early Career Committee (SECC) since the pandemic began and we are grateful to all those that have travelled to be with us today in the vibrant city of Birmingham. Given Birmingham is known as the birthplace of the Industrial Revolution it is somewhat fitting that we come together today thinking about the Sustainable Revolution and the future direction of materials, minerals and mining research.

We have an exciting programme lined up that will allow delegates to explore current and future research directions, reflect upon and celebrate recent accomplishments, renew friendships and extend our networks. We hope that you have a productive and enjoyable time at this very special conference.

This conference series, organised by the Institute of Materials Minerals and Mining (IOM3) SECC, is intended to be a forum for early career materials, minerals and mining scientists and engineers from across the UK to come together and present their research on the materials they are developing and working with, with the hope of improving presentation skills, along with initiating collaboration between research groups, and between industry and academia. It is also a way of helping researchers and industry workers see how their work fits into the bigger picture of future materials, minerals and mining research and technology across the UK. With this in mind, we encourage open and friendly discussions, networking and hopefully a number of future collaborations!

To put together a conference is no small task so we must extend our thanks to the members of the Committee (past and present) that provided their time and effort, also a great many thanks are extended to the IOM3 team whose support was invaluable. We would of course like to thank all of the sponsoring organisations for providing their generous financial support which allows us to keep this conference free of charge to our delegates. Lastly, we would like to thank all of the conference participants for their contributions which are the foundation of this conference.

Dr Ilija Rašović MIMMM **Conference** Chair

Martyn Jones CEng MIMMM SECC Chair



Student & Early Career Committee

The SECC represents the views of student, younger and early career* members to the Institute's Executive Boards and Advisory Council. We aim to represent the diverse range of members by ensuring Council representatives cover the different disciplines, regions and career pathways of student and early career members.

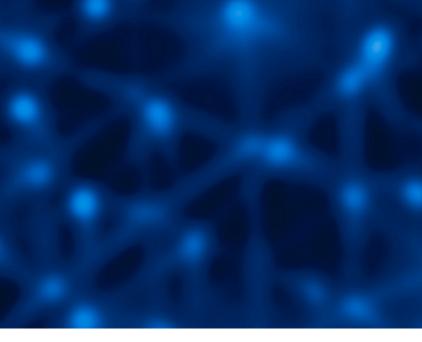
Since the Committee was founded in 1967 (as the Younger Members' Committee), we have developed a range of events to encourage networking and early career members' involvement with IOM3. Our greatest successes to date include the Young Persons' Lecture Competition, Matopoly, Professional Development events and Future Materials Conference. While we have been successful in the past, we aim to provide more events in the future. These include regular informal networking opportunities, along with new skills seminars, conferences and regional events.

* The Institute defines 'early career' as meaning someone who is, as of 1 September 2020 (and allows for career breaks, e.g. parental leave):

- 1. within 10 years of the start of their first employment (or self-employment) in a materials, minerals or mining related role, or
- 2. within 6 years of completing their PhD (in a relevant subject), whichever is sooner.

Note - the 10 years from the start of first employment would not normally include any apprenticeships (or equivalent training scheme).

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The Henry Royce Institute is the UK's national institute for advanced materials research and innovation. Royce was established to ensure the UK can exploit its world-leading expertise in advanced materials and accelerate innovation from discovery to application. With investment of over £330 million from the Engineering and Physical Sciences Research Council (EPSRC), Royce is ensuring that both the UK academic and industrial materials community have access to world-class research capabilities, infrastructure, expertise, and skills development.

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MIDAS

THE MIDAS PROGRAMME...

...benefits from a unique set of industrially-relevant materials irradiated in a research reactor to very high fluence levels, which were contributed to the research team by Westinghouse and the international Nuclear Fuel Industry Research (NFIR) programme. Due to their unique nature these samples have significant worth, which, alongside core funding from the Engineering and Physical Sciences Research Council (EPSRC) industrial commitments, bring the total value of the programme to around £25 million.

The assembly materials studied are those used as protective cladding for the highly radioactive fuel used in a nuclear reactor. Due to the need to operate reactors as safely as possible, fuel is often removed well before it is spent (i.e. before all the energy is extracted) because not enough is currently known about these cladding materials, so plant operators must adopt a highly cautious, safety-first approach. This reduces the cost-efficiency of nuclear power as an energy option, as well as meaning that the fuel assembly prematurely becomes additional waste, which must be safely handled and stored over the long term.

Reactor safety, however, remains paramount, so MIDAS also has a dedicated work package, within Key Challenge 4, on better understanding fuel cladding behaviour in accident scenarios. The aim of this is to ensure that reactors remain safe in the event of an incident such as Fukushima, as well as including work on the development of accident-tolerant fuels.

A further key theme of MIDAS is to explore the use of zirconium alloys in critical components for future fusion reactors. The UK has a leading position in defining the materials that will be chosen for the ITER and DEMO international fusion projects, and this theme will contribute to maintaining the UK's reputation as a centre of excellence in fusion research.

Central to the programme is the use of UK facilities at which work on active samples may be undertaken. These include National Nuclear User Facility sites at the National Nuclear Laboratory, Materials Research Facility and The University of Manchester's Dalton Cumbrian Facility, as well as new capabilities made available through the Henry Royce Institute. These have received significant investment from the UK government, and MIDAS is a key beneficiary of this investment, as well as being a trailblazing project to showcase what research is possible at these new and enhanced facilities.

The ultimate goal of MIDAS is to help the UK, and other countries, meet carbon reduction targets, and achieve an energy mix that produces less CO2. The MIDAS team is therefore working closely with a range of UK and international industrial partners and stakeholders in addressing this challenge and translate fundamental research into real-world impact.

zr-midas.org

Future Materials Conference

10.00	Registration/coffee
10.30	Welcome Dr Ilija Rašović MIMMM, Conference Chair
10.40	Keynote 1
	Neofossils: Bio-based plastics to sequester CO₂ Prof Anthony J Ryan OBE, Director, The Grantham Centre for Sustainable Futures, The University of Sheffield
	Session 1
11.10	Using bridging flocculation for the development of a polymer-based point of care diagnostic for targeted detection of bacterial DNA Elisabeth Trinh* & Lee Fielding (University of Manchester)
11.25	Man-made crystals for jewellery Sofie Boons (University of West England)
11.40	The use of interleaved films to optimise the production of all-cellulose composites using textile waste Ashley Victoria MEng, MSc (University of Leeds)
11.55	Break
	Keynote 2
12.05	Materials and Design Exchange (MaDE): Helping to commercialise metamaterials Dr Robert Quarshie, KTN Head of Materials & MaDE Chairman
	Session 2
12.35	Exploiting the elastic properties of metallic glasses Osama Shahin Elzoubi PhD*, Martin Stiehler & Konstantinos Georgarakis (Cranfield University)
12.50	DFT exploration of the family of 2D metal organic frameworks M(C4N2H4)C12 Andrea Iliceto (University of Birmingham)

1.05	Artificial neural networks for high throughpu Jordan Dorrell* & Andrew Morris (University o
1.20	Modelling amorphous zirconia using density Christopher Owen (University of Birmingham)
1.35	Lunch
	Session 3
3.00	Making the most of your IOM3 Membership Sarah Boad, Membership Development Manag
3.30	Keynote 3
	You never know until you ask Dr James Perkins CPhys, Queen Elizabeth's Gr
4.00	Improving sustainability in the aluminium ind Dr Michael Kenyon MPhys, PhD (Innoval Techr
4.15	Understanding local microstructural evolutio bed infusion additive manufacturing Anna Tholen*, Rebecca Higginson, Lewis Jone
4.30	Importance of electronic correlations for the Dr Hrishit Banerjee* & Marcus Aichhorn (Unive
4.45	Multi-scale in situ studies of deformation mea Wanxuan Teng* & Biao Cai (University of Birm
5.00	Closing remarks
	Dr Ilija Rasovic MIMMM, Conference Chair Martyn Jones CEng MIMMM, SECC Chair
5.15	End



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Programme in brief

10.00 Registration/coffee

10.30 Welcome Dr Ilija Rasovic MIMMM, Conference Chair

10.40 Keynote 1

Neofossils: Bio-based plastics to sequester CO₂ Professor Anthony J Ryan OBE Director, The Grantham Centre for Sustainable Futures, The University of Sheffield

In the last 50 years more than 8 billion tons of the stuff vilified as "plastic" has been produced. The ingenuity of polymer scientists & engineers, plus the ubiquity and variety of polymers, mean they are completely embedded in our lives. But the very properties of plastics that make them so useful, they are durable & cheap, also means that they almost worthless post-use, expensive to recycle & easy to discard.

We have been focussed on delivering a circular economy for polymers, whether they are derived from fossil carbon or more recent biomass. A systems-based, multidisciplinary approach can solve the problem of plastics in the environment through a combination of reuse, repurposing & recycling. This work has led us to the conclusion we need to turn the problem on its head. Make more single use plastic but using C that has been fixed by photosynthesis and taken from the atmosphere this year, not C fixed millenia ago. Neo-carbon not fossil-carbon to turn into neo-fossil plastic and put it back in the ground through curated burial.

The current emphasis on bio-based & compostable plastics is not inherently sustainable because their production can cause more greenhouse gas emissions than the fossil-based plastics they replace. Moreover, the fate of a compostable plastic is conversion back into CO2 & water. Bio-based plastics can only become truly sustainable when produced using renewable energy, not the current energy mix of >80% fossil. Life cycle assessment can identify the tipping point, as the energy system defossilises, when making durable bio-based plastics makes sense.

The Intergovernmental Panel on Climate Change (IPCC) has a 1.5 °C target with a commitment to the removal of 12 billion tons of CO2 per year, >25% of current emissions, yet there are no scaleable technologies to do this. Herein lies an opportunity It could turn plastic consumption into a good thing, the environmental benefits of plastic (reduced food waste being one example) could be maintained.

The petrochemicals industry could continue to benefit from its capital assets and be persuaded to leave the oil & gas in the ground if it could see a profit from a "consume then conserve" plastic policy.

When plastic sequesters carbon from the atmosphere by being made from biomass it makes sense to use it to replace even more materials. For example carbon fibre composites (where both the fibre & the resin were neocarbon) could replace lightweight metals in transport and steel in construction.

We could use durable (i.e. nondegradable) bioplastics plastics to sequester carbon. Making polymers from photosynthetic biomass takes CO2 out of the atmosphere and we could bury that plastic. In fact, if we converted all the current 300 million tonnes of annual plastic production to non-degradable bioplastics, using 100% renewable energy and agricultural waste as the feedstock, we would be able to remove 1 billion tonnes of CO2 from the atmosphere every year.

Session 1

11.10 Using bridging flocculation for the development of a polymer-based point of care diagnostic for targeted detection of bacterial DNA Elisabeth Trinh* & Lee Fielding (University of Manchester)

There is an unmet clinical need for a fast and cost-effective point-of-care diagnostic for the presence of a bacterial infection in patient samples. For example, the unnecessary use of antibiotics is a significant contributor to the catastrophic rise in antimicrobial resistance seen today. The current gold standard diagnostic for bacterial identification is time consuming and requires an expert / analytical lab to perform the test, taking up to five days for results to be reported. This presentation outlines the steps taken to develop a rapid and cost-effective alternative, reducing the time taken to identify bacterial infections from five days to two hours, whilst avoiding specialist equipment or expertise. Our strategy is based on the use of charge complexation and bridging flocculation in order to detect the presence of amplified DNA. Specifically, we have designed and synthesised sterically-stabilised, polymer latexes which we use to indicate the presence of DNA with a relatively high molecular weight. If DNA is present in a given sample, the anionic DNA backbone complexes with the latex particles and induces flocculation followed by rapid sedimentation, thus giving a clear visual result.

11.25 Man-made crystals for jewellery Sofie Boons (University of West England)

With crystal growing techniques having been around for many years, bespoke man-made crystals now drive innovations in a range of industries. This has however not translated into the jewellery industry, where innovations with man-made crystals have remained limited, and most are still produced to replicate mined crystals. My PhD study will therefore investigate the design implications, possibilities and limits of utilising man-made crystals in the development of jewellery designs. Whilst conducting experiments and developing planned collaborations the changing role of the designer will also be explored in relation to the amount of control and input the designer has had in the material development stage. Finally, the appreciation of these man-made crystals and the context in which they are appraised will be explored as part of the contextual review.

11.40 The use of interleaved films to optimise the production of all-cellulose composites using textile waste

Ashley Victoria MEng, MSc (University of Leeds)

All-cellulose composites (ACCs) have attracted significant attention within the research community in recent years as a sustainable alternative to traditional multi-component composites. In this context, ACCs are composites where

both fibre and reinforcement are comprised entirely of cellulose, a naturally occurring biopolymer with inherently strong mechanical properties. Having chemically identical components gives ACCs an advantage over traditional fibre reinforced polymer composites, or natural fibre reinforced composites (NFRCs) where recycling mixed material components can be challenging. This work introduces a novel route for producing ACCs with enhanced interlaminar adhesion between multiple layers. By combining textile reinforcement with interleaved films, this process overcomes the issue of insufficient matrix production that can lead to common failure mechanisms such as delamination. CCs were produced by partially dissolving alternating layers of cotton textile and cellulose film in solvent solution and heating them under compaction. After heating, the samples were placed in a water bath allowing the dissolved cellulose fraction to coagulate, forming a solid material. The solvent used in this study was ionic liquid 1-ethyl-3-methylimidazolium acetate (EMIMAc) combined with dimethyl sulfoxide (DMSO). Mechanical properties of the resulting composites such as tensile strength and Young's modulus were determined, as well as peel strength, which is a measure of adhesion between layered structures. Influence of interleaf film and dissolution time were initially investigated, with subsequent exploration of the ratio of EMIMAc to DMSO in solution. The results showed that the addition of interleaf film yielded a significantly higher peel strength compared to processing without the film, and an optimum processing time that is favourable for an industrial process. In addition, there was improved uniformity of mechanical properties between in-plane and transverse directions.

11.55 Break

Keynote 2

12.05 Materials and Design Exchange (MaDE): Helping to commercialise metamaterials Dr Robert Quarshie KTN Head of Materials & MaDE Chairman

By exploiting the physics, chemistry and microstructural properties of an array of engineered materials, metamaterials can be produced with properties never found in nature and of great potential commercial value. There are a wide range of potential applications and the power to transform the way we do things in important areas, from energy to ICT, defence & security, aerospace, and healthcare, to name but a few. Metamaterials can be engineered to bend light to create an invisibility cloak and absorb sound waves to reduce excessive noise or generate complete silence.

Metamaterials have their roots in the work of radar engineers in the second world war and reinvigorated by the research of some of our most senior academics, including Professor Sir John Pendry of Imperial College London. Despite the UK being a global leader in academic research in this area we lack large scale industrial uptake for commercial applications. These materials are not easy to understand and require the creation of novel supply chains. Recent collaboration with the design community, helped by the Materials and Design Exchange (MaDE), is beginning to generate the type of business interests required to exploit the £10bn of potential growth for metamaterials globally.

Dr Robert Quarshie will present the work of the Metamaterials Innovation Network and what has been achieved in collaboration with MaDE.

Session 2

12.35 Exploiting the elastic properties of metallic glasses Osama Shahin Elzoubi PhD*, Martin Stiehler & Konstantinos Georgarakis (Cranfield University)

Unlike crystalline metals, metallic glasses do not have a periodic lattice with glide planes on which mobile dislocation can cause plastic flow. Consequently, they

show a wide elastic strain range on the order of 2% before the onset of plastic deformation which occurs in a highly localized manner on planes of maximum shear stress. Their exceptional mechanical properties lead to a unique and reversible sinusoidal mechanical response of metallic glass foils that are elastically shaped to form an arc. Under a normal load applied on the top of the sinusoidal arc, the foil deforms elastically leading to the successive formation of sinusoidal wavy patterns of higher order. The non-linear load versus displacement response allows metallic glass foils to act as a non-conventional spring with variable equivalent spring constants at different ranges of applied load. This recently discovered mechanically induced undulatory behaviour of metallic glasses, resulting from their exceptional buckling response, offers new opportunities for exploring novel functionalities of metallic glasses in a wide range of applications including micro-springs, sensors and actuators, shock absorbance and energy harvesting.

12.50 DFT exploration of the family of 2D metal organic frameworks M(C₄N₂H₄)C₁₂ Andrea Iliceto (University of Birmingham)

Metal organic frameworks are a class of microporous coordination polymers which are growing in popularity thanks to their vast application potential, such as gas storage, filtration and sensing, as well as catalysis. Searching for new structures and exploring their characteristics has traditionally been a complex experimental objective, but with the growing accuracy of computational techniques, studying novel MOF structures has become more efficient and lowered research costs. This computational exploration has explored the structure and properties of a new family of 2D metal organic frameworks, $M(C_4N_2H_4)C_{12}$, where M = transition metals V to Cu. An overview of the different computational approaches will be presented, including DFT+U, transition metal swaps and symmetry breaking. The importance of adding a Hubbard U correction to treat the strong on-site Coulomb interaction of localized electrons, which is not correctly described by LDA or GGA, has been found to increase the band gap around the Fermi level. This presentation will also give an insight into the practical secrets of carrying out computational research with MOFs, including the manipulation of spin

states via the breaking of spin symmetry of the system, as well as understanding the possible ferromagnetic and antiferromagnetic output configurations that may arise. This research aims at progressing this exciting field of science in which the organic and inorganic worlds come together to offer a future of great potential applications.

13.05 Artificial neural networks for high throughput material discovery Jordan Dorrell* & Andrew Morris (University of Birmingham)

Artificial neural networks (ANN) are becoming increasingly popular in many fields of research across the globe. One such example of the success of ANNs has been in the field of atomistic modelling where machine learning potentials (MLPs) have been used to bridge the gap between highaccuracy ab initio calculations and high-speed molecular mechanics calculations. We have used an iterative method to train continuous-filter convolutional ANNs on an (initially) small data set compromising density-functional theory (DFT) data. The resultant MLPs were used to perform the geometry optimisation step of a random structure searching method. DFT calculations were then performed on the optimised structures. By these means, we reproduce the accuracy of the ab initio random structure searching method, but at a lower computational cost. We have used the method, which we term machine learning random structure searching, to explore the Li-Ni-S ternary phase diagram in search of a new high-capacity cathode material.

13.20 Modelling amorphous zirconia using density functional theory

Christopher Owen (University of Birmingham)

Developing rechargeable batteries with greater charge capacity is an important aim for the future of electronic vehicles and devices, however it is difficult to overcome electrode degradation. Metal oxide coatings have been found to improve performance and inhibit degradation of battery electrodes during cycling. These coatings are often amorphous, which makes them difficult to structurally characterise. To design successful coatings, it

is important to understand electronic properties and ion transport through the material. Atomistic modelling can be used to enhance experimental approaches by correlating spectroscopy data with atomic structure. DFT enables properties of materials to be calculated without requiring empirical data, and so can be used to make accurate predictions for unknown systems. In this work, amorphous zirconia structures were generated using ab initio molecular dynamics (AIMD) with a melt-guench technique on 96 atom cells. As the true density of amorphous zirconia is not clear, the cells had densities ranging from 4.8-6.0g/cm^3. These structures were characterised by their pair distribution functions (PDFs), coordination environments and calculated O and Zr NMR chemical shifts, with the aim of fingerprinting the structures such that they can be validated against experimental data. It was found that coordination numbers in the structures generally increased with density, which suggests NMR spectroscopy could be used to narrow the density range significantly.

13.35 Lunch

Session 3

15.00 Making the most of your IOM3 Membership Sarah Boad Membership Development Manager, IOM3

15.30 Keynote 3

You never know until you ask Dr James Perkins CPhys Queen Elizabeth's Grammar School

Where do we get the next generation of colleagues in academia and industry? The materials cycle is met in many areas of the school curriculum yet specific careers and vocations within the industry is largely unknown in many schools. Seconday education needs inspirational people to be visible and relatable to the young people who are making life changing decisions on their future at a really young age.

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Targeted outreach and public engagement should not be an add on but an integrated part of what all scientists do in order to raise the scientific capital of a population. The SEM in schools project is an example of where 'deep impact' outreach can inspire, engage and ultimately help raise the calibre and diversity of the materials cycle workforce. This can only happen when teachers and scientists work together as equals and a mutual respect is formed through shared activities and innovation both in education and research.

16.00 Improving sustainability in the aluminium industry Dr Michael Kenyon MPhys, PhD (Innoval Technology)

Every material sector is facing increased pressure from consumers to governments to improve its environmental impact with legislative targets introduced for many industries across the world. Future materials will have to be not only designed, but eco-designed, with recyclability considered at an early design stage. This includes the metals industry and more specifically, the aluminium industry which currently accounts for around 2% of global Green House Gas (GHG) emissions alone. The aluminium industry is forecast to grow rapidly, while at the same time, aiming to reduce its overall environmental impact. This talk introduces the environmental hotspots along a typical aluminium supply chain, and how the sustainability performance can be improved. Three main areas are discussed in the improvement of the industries environmental footprint, including: (1) decarbonising its energy supply, (2) increasing the recycling rate of end of life materials, and (3) increasing the recycled content within new aluminium products among other potential options. These options are discussed within some of the major aluminium markets, transport, packaging and construction sectors.

16.15 Understanding local microstructural evolution in tool steel processed by laser powder bed infusion additive manufacturing

Anna Tholen*, Rebecca Higginson, Lewis Jones, John Tyler & Nick Jones (Loughborough University)

Hot-work tools steel alloys rely on complex changes and developments to their microstructures during heat treatment to optimise the mechanical properties. In their optimised state, tool steels exhibit excellent wear resistance, good thermal fatigue properties and corrosion resistance making them the material of choice for hot working and cutting tools across a number of manufacturing processes. These properties are achieved by the formation of martensite and hard carbide particles within the microstructure. Laser powder bed fusion (LPBF) additive manufacturing (AM) is an increasingly popular process for the manufacture of steel components, especially for tool steel alloys. When processed by subtractive processes, tool steels require machining in a softened state as the final wear resistance often matches those of cutting tools involved in the process. However, the rapid and cyclical heating and cooling of the LPBF AM process has been shown to make them more brittle and susceptible to defect propagation. This means that the performance of tool steel components built by LPBF AM can be inferior to their conventionally processed counterparts. This research investigates how local microstructural evolution changes throughout the build material and discusses how this links with mechanical properties and susceptibility to defects such as cracking. This research uses advanced material characterisation techniques to examine the local microstructure properties such as grain morphology and misorientation behaviour throughout H13 samples processed by LPBF AM.

16.30 Importance of electronic correlations for the magnetic properties of 2-dimensional ferromagnets Dr Hrishit Banerjee* & Marcus Aichhorn (University of Cambridge)

We investigate the emergence of ferromagnetism in twodimensional metal-halide CoBr2, with a special focus on the role of electronic correlations. The calculated phonon spectrum shows the exfoliated system is thermodynamically stable. We apply two well-known methods for the estimation of Curie temperature. First, we do DFT+U calculations to calculate exchange couplings, which are subsequently used in a classical Monte Carlo simulation of the resulting Ising spin model. The transition temperature calculated in this way is in the order of 100K, but shows a strong dependence on the choice of interaction parameters. Second, we apply dynamical mean-field theory to calculate the correlated electronic structure and estimate the transition temperature. This results in a similar estimate for a noticeable transition temperature of approximately 100K, however, without the strong dependence on the interaction parameters. The effect of electron-electron interactions are strongly orbital selective, with only moderate correlations in the 3 low energy a1g+eg- π orbitals, and strong correlations in the higher energy eg- σ orbitals. This can be traced back to the electronic occupation in DMFT, with five electrons in the three low-lying orbitals (a1g+eg- π) and two electrons in the eg- σ , making the latter one half-filled. Nevertheless, the overall spectral gap is governed by the small gap originating from the low-lying a1g+eg- π orbitals, which changes very weakly with interaction U. In that sense, the system is close to a Mott metal-to-insulator transition, which has been shown previously to be a hot-spot for strong magnetism. Ref.: Phys. Rev. B 103, 195123 (2021)

16.45 Multi-scale in situ studies of deformation mechanism of L-PBF 316L stainless steels Wanxuan Teng* & Biao Cai (University of Birmingham)

An understanding of deformation mechanisms of laser powder bed fusion (L-PBF) 316L stainless steels was important for further optimization of LPBF processing and the in-service applications of L-PBF 316L steel. In this study we used in situ synchrotron characterization to study the formation of corrugated surface in L-PBF 316L stainless steel during mechanical loading. In situ tomography analysis was carried out revealing the surface morphology and porosity evolution. The pores elongate and reaching the surface during loading. A corrugated surface was formed after plastic deformation. Ex situ characterisations including optical microscopy and electron microscope revealed the microstructures contributed to the mechanical performance. The findings show the further need to optimize the mechanical performance of additive manufactured alloys through tailoring the microstructure.

17:00 Closing remarks

Dr Ilija Rasovic MIMMM, Conference Chair Martyn Jones CEng MIMMM, SECC Chair

17:15 End

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