





# Student Conference in metallic

materials

Organised by the EPSRC and SFI Centre for Doctoral Training in Advanced Metallic Systems

11 – 12 July 2022 The Helix Dublin City University











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#### **Monday 11th July**

#### 9:00 Registration & Refreshments

#### 9:30 Welcome – Gallery Room

Professor Dermot Brabazon, AMS CDT ROI Director, Dublin City University **Keynote** 

Dr Nesma T. Aboulkhair, The University of Nottingham 'Metal Additive Manufacturing: From Loose Powder to Complex 3D Structural and Functional'

#### 10:20 Parallel Session 1

1A – Gallery Room Advanced Processing and Characterisation

Chairs: Lucy Farguhar & Sam Lister

10:25 Development of Advanced High Modulus Steels for Automotive Applications

Sully Khan, The University of Sheffield

10:40 Additive Manufacturing for the Development of Microneedle Arrays as Minimally Invasive Drug Delivery Systems

Nikoletta Sargioti, Dublin City University

10:55 Order-Disorder Transformation Control in AlTiVCr-Based High Entropy Alloys

Panagiotis Stravroulakis, The University of Sheffield

11:20 Refreshment Break - Atrium

#### 12:00 Parallel Session 2

2A - Gallery Room Microstructural Design

Chairs: Joshua Collins & Ashley Scarlett

1B - Blue Room Corrosion and Surface Engineering

Chairs: Sakina Zaman & Huda Al-Jurani

Producing Precious Metal Doped Stainless Steels by Spark Plasma Sintering

Natasha Sweeney Fort, The University of Sheffield

Understanding the Effect of Strain on Microstructure Properties and Environmental Degradation of AGR Fuel Cladding

Alexander Hanson, The University of Manchester

The Use of Nanosecond Pulsed Laser Modification for the Increased Lifetime of a Commercially Used Pulsed Electric Field (PEF) System Mark Swayne, Dublin City University

2B - Blue Room Alloys & Brazing

Chairs: Frances Livera & Xavier Sanuy Morell

#### 12:05 Spreading Area Measurements of Sn-Ag-Cu Lead Free Solder on Silver and **Copper Substrates**

Wunmi Olukoya, The University of Sheffield

#### 12:20 The Evolution of Microstructure and **Toughness in Multipass Welds that Contain Acicular Ferrite**

Enn Veikesaar, The University of Manchester

#### 12:40 Modelling the Microstructure **Evolution of Titanium Alloys**

Guy Bowker, The University of Manchester

**Tool Wear in CVD Coated Carbides** when Machining Ni-based Superalloys Henry Boyle, The University of Sheffield

#### In Situ Characterisation of the **Thermomechanical Deformation Behaviour of Powder Processed Ni**based Superalloys

Frances Synnott, The University of Sheffield

**Characterisation of Zirconium Alloys** with Copper and Vanadium Additions for Nuclear Fuel Assembly Materials Callum Andrew, The University of Manchester

#### 13:00 Lunch and Poster Presentations - Atrium

#### 14:30 Keynote – Gallery Room

Professor Andrew Parnell, Maynooth University 'Anomaly Detection and Other Machine Learning Tools in Industry 4.0'

#### 15:20 Parallel Session 3

#### 3A - Gallery Room **Demanding Environments & Energy** Chaired by Sakina Zaman & Kavi Sharma

#### 15:25 **Development of an Optical Fibre Mid-Wave Infrared Thermometer for Metal Machining Operations**

Emilios Leonidas, The University of Sheffield

#### **Computational Study of Microstructurally** 15:40 **Short Crack Propagation in AA7XXX Alloys**

Cameron Grant, The University of Manchester

#### Modelling the Behaviour of Irradiation-15:55 **Induced Defects in Nuclear Zirconium**

Jake Larkin, The University of Manchester

#### 3B - Blue Room **Machine Learning & Data Analysis** Chaired by Anesu Nyabdaza & Bryan Naab

#### Measuring Image Quality of 3D X-Ray **Computed Tomography**

Jamie McGregor, The University of Manchester

#### **Design of HEA Hardmetals for Tooling Applications**

Joshua Berry, The University of Sheffield

#### **Anti-Ice Fouling Surfaces by Fabrication Superficial Structures on Aluminium** Alloys by Laser Machining

Abhijit Suhas Cholkar, Dublin City University

#### 16:10 Refreshment Break - Atrium

#### 16:40 Ultrashort Laser Sintering of Metallic Nanoparticle Inks on Heat Sensitive Substrates

Ayesha Sharif, National University of Ireland Galway

### 16:55 Effect of Microstructure on the Localised Corrosion of 15-5PH Stainless Steel

Alyshia Keogh, The University of Manchester

### Molecular Dynamics (MD) Simulation of TWIP/TRIP Metals and Alloys

Mehran Bahramyan, Dublin City University

### Microstructural Fingerprinting via Variational Autoencoders

Mike White, The University of Sheffield

#### 17:15 Drinks Reception – Atrium

#### **6pm Coach departs for transfer to Conference Dinner**

#### **Conference Dinner and Irish Dancing Experience**

Arlington Hotel, 23-25 Bachelors Walk, O'Connell Bridge, Dublin 1

A 3-course menu will be served.

Starter options: Duck Salad, Soup, Prawn Salad or Cantaloupe Melon

Main options: Irish Lamb Stew, Boiled Bacon, Chicken Supreme, Salmon, Bean Chilli,

or Beef & Guinness

The coach will depart The Arlington at 10.30pm to return delegates to their hotels.



#### **Tuesday 12th July**

#### 9:00 Refreshments & Posters - Atrium

#### 9:30 Welcome – Gallery Room

Professor Russell Goodall, AMS CDT UK Director, The University of Sheffield **Keynote** 

Professor Claire Davis, Warwick Manufacturing GP at The University of Warwick 'Rapid Alloy Development for Sustainable Steels'

**Announcement** by Dr Richard Dawidek, Royce at the University of Sheffield, on 'Royce Researcher & Student Equipment Access Schemes'

#### 10:20 Parallel Session 4

#### 4A - Gallery Room Modelling and Simulation

Chairs: Guy Bowker & Mike White

# 10:25 An Investigation into the Effect of Microtextured Regions on the Fatigue Properties on Forged Titanium

Patrick Curran, The University of Manchester

### 10:50 The Development of a Rapid CCT Predictor for Low Alloy Steels

Joshua Collins, The University of Manchester

# 11:10 The Influence of Prior Deformation and Creep Asymmetry on Stress Relaxation and FE Modelling of Creep Age Forming AA2139 Plate

Kevin Tanswell, The University of Manchester

#### 11:20 Refreshment Break - Atrium

#### 12:00 Parallel Session 5

#### 5A - Gallery Room Modelling and Simulation

Chaired by Joshua Collins & Frances Livera

#### Session 4B - Blue Room Additive Manufacturing & Sustainability

Chairs: Lucy Farquhar & Nikoletta Sargioti

### **3D Printing of Continuous Stainless-Steel Fibre/Polymer Composites**

Alison Clarke, University College Dublin

#### Methodologies Used in the European Countries for Critical Raw Material Assessment

Ahmar Murtaza, Dublin City University

# Pulsed Laser Ablation in Liquid for the Fabrication of Magnesium and Carbon Nanoparticle Inks

Anesu Nyabdaza, Dublin City University

5B - Blue Room
Additive Manufacturing &
Sustainability

Chaired by Vincent Kan & Josiah Chekotu

#### 12:05 Coupling Component Diffusion with the Precipitation Kinetics of Ni-Based Superalloys

Sakina Rehman, The University of Manchester

12:20 Modelling the Effects of Texture on the Stress and Strain Localisation During Bending of Aluminium Alloy Sheet Laura Gonzalez Duque, The University of Manchester

Influence of Solution Heat Treatment
Temperature and Holding Time on the
Microstructure, Texture, and Hardness of
IN718 Produced by the L-PBF
Merve Nur Dogu, Dublin City University

Microstructural Influence on the Fatigue Behaviour of Additively Manufactured Ti64 Alloy

Bryan Naab, University College Dublin

### 12:40 Closing Session - Gallery Keynote

Declan Bourke, Product Development Manager, Fort Wayne Metals 'Nitinol Processing and Applications - Current State of Arts, Trends, and Challenges'

Poster & Oral Presentation Prize Awards – Professor Russell Goodall

13:30 Lunch - Atrium

15:30 Coach transfer to airport

#### **Keynote Speakers**

### Metal Additive Manufacturing: From Loose Powder to Complex 3D Structural and Functional Products

Dr Nesma Aboulkair, The University of Nottingham **Biography** 

Dr Nesma Aboulkhair works in metal AM using various technologies, such as using droplet-on-demand technologies (Metal Jet) to jet high temperature electrically conductive molten metals into micron-scale features. Her projects span a range of alloys using powder-based laser AM technologies, focussing on the process-structure-property relationships, incorporating extensive experience in parameters optimisation and control for successful fabrication of defect-free parts and characterisation of the microstructural and mechanical behaviours.



#### **Abstract**

Metal additive manufacturing is strongly positioning itself as a predominant player in today's manufacturing landscape. With the unmatched degrees of freedom this family of manufacturing processes warrant, fabricating sophisticated components that was otherwise unachievable has become possible. This talk will give an overview of the recent advances in metal additive manufacturing activities currently taking place at the newly established. Additive Manufacturing laboratory at the Technology Innovation Institute (TII) in the UAE. Focussing on the process-structure-property relationships in metal additive manufacturing via laser powder bed fusion, our research avenues include 3D Printing of high-performance metals, next generation materials for laser powder bed fusion, and redesign via additive manufacturing to exploit the potential of light-weighting and engineering bespoke mechanical performances.

#### **Anomaly Detection and Other Machine Learning Tools in Industry 4.0**

Professor Andrew Parnell, Maynooth University

#### **Biography**

Andrew is Hamilton Professor in the Hamilton Institute at Maynooth University. His research is in statistics and machine learning for large, structured data sets in a variety of application areas. He has co-authored over 75 peer-reviewed papers and has been involved in grants totalling over €65 million as PI/collaborator. He has been heavily involved in the commercialisation of research through the start-up companies Prolego Scientific and Atturos. He is currently a principal investigator in the SFI I-Form Advanced Manufacturing Centre, and a funded investigator in the SFI Insight Centre for Data Analytics.



#### **Abstract**

Many processes which fall under Industry 4.0 provide the operator with an enormous amount of data for every manufactured part. It can be very hard to reason with data sets of this size and dimension, let alone make informed decisions about whether a part has been produced to a desired quality level. In this talk, I will provide a tour of some of the methods developed and used by the I-Form Centre for Advanced Manufacturing (www.i-form.ie). I will explain how some of these machine learning tools work, and how they can be used to identify anomalies in real time for an additive manufacturing process.

#### **Rapid Alloy Development for Sustainable Steels**

Professor Claire Davis, The University of Warwick **Biography** 

Professor Claire Davis holds a RAEng / Tata Steel Chair in Low Energy Steel Processing and is the Head of the Advanced Steel Research Centre (ASRC) in WMG, University of Warwick. The ASRC focusses on fundamental and applied research from steelmaking to final product and is a group of over forty researchers. Professor Davis's personal research interests are on the development of microstructure during processing and the relationships between microstructure and properties (both physical and mechanical) in steels. She also works on non-destructive evaluation of microstructure



#### **Abstract**

using electromagnetic sensors.

How can the academic community support the rapid development and adoption of new steels and processes in the steel industry? The drive to lower CO<sub>2</sub> emissions means that there are changes occurring in the steel industry, which include introduction of new steelmaking processes and an increase in recycling as well as the continued demand for improved steels. To support these changes, for example through considering the implication of increased residual elements from recycling and to develop new steels / processes laboratory facilities and modelling need to be capable of replicating industrial processing. In this talk rapid alloy processing for steel will be discussed, with examples of how industrial process parameters are considered and how residual elements affect the steels' microstructure and properties.

### Nitinol Alloy Processing and Applications – Current State of Art, Trends, and Challenges

Declan Bourke, B.E. (Mech), M.Eng. Sc., Product Development Manager, Fort Wayne Metals Ireland **Biography** 

Declan is currently undertaking a PhD on laser bed powder fusion nitinol on a part-time basis, at the department of mechanical engineering at DCU. Declan has worked for the past 17 years at FWMI in various process engineering, quality engineering and R&D roles. Fort Wayne Metals is a leading manufacturer of metal products for medical devices and high specification industrial applications. The company has evolved to a fully integrated system of melt, production, and across 17 facilities in the U.S. and Ireland.



#### **Abstract**

FW Metals offers a range of alloys – including NiTinol, titanium, cobalt chromes, stainless steels, and high-performance alloys – for a wide spectrum of materials and forms, including round wire, shaped wire, bar, rod, sheet, strands, cables and assemblies. These products are for use in a wide range of medical devices such as cardiovascular, neurostimulation, orthopaedic and orthodontic applications, as well as a number of high specification automotive, aerospace and general industrial applications. One of the fastest growing alloys in terms of demand and range of applications is nitinol. An overview of current state of the art processing of nitinol, its properties and applications are covered in this presentation. Challenges and limitations are identified with respect to current subtractive manufacturing processes, and challenges and opportunities are identified regarding Additive Manufacturing (AM) for production of high specification nitinol components.

#### Posters at a glance

1. Advancing Gear Oil Insights: Tribofilm and Subsurface Correlation Focusing on Ashless Versus Organometallic Chemistries

Ashutosh Gupta, The University of Manchester

2. Assess Hydrogen Embrittlement Behaviour by Investigating the Impact of Different Electrochemical Charging Levels Through the Bulk Steel Specimen

Mehreen Kainat Khan, The University of Manchester

3. Assessment of Local Ordering in the NiCoCr Ternary Alloy Down to Low Temperature via Total Scattering Analysis

Benjamin Jolly, The University of Sheffield

**4.** Characterisation and Thermodynamic Modelling of Mg-Zn-Gd-Zr Variant Alloys Sian Odell, The University of Manchester

5. Creation of Digital Fingerprints from Machining Force Feedback Data

Joshua Taylor, The University of Sheffield

 Development and Characterization of Calcium Phosphates Coating Layers on Magnesium Substrates for Control the Degradation Rate and Enhance the Bone Repair for Potential Orthopaedic Implantation Applications

Tina Sadat Hashemi, Dublin City University

7. Development of New Beta-Titanium Alloys for Additive Manufacturing of Biomedical Implants
Theo Mossop, University College Dublin

8. Effect of Heat Treatment on the Performance of Nitinol Wires for Actuators

Josephine Ryan Murphy, Dublin City University

9. Environmental Impacts of Alternative Blast Furnace Ironmaking Materials

Siti Nurlisa Ahmad, The University of Sheffield

10. Estimation of Fracture Toughness for Ferritic Steels in the Transition Range

Kamila Nowosad, The University of Sheffield

11. Experimental Analysis of R-Phase NiTi Tube Actuators Using Conductive/Convective Heating Stage

Lehar Asip Khan, Dublin City University

12. Finite Volume Simulation of Extrusion Processes

Ali Shayegh, University College Dublin

13. Heat Treatment of Nitinol Manufactured via L-PBF for Biomedical Applications

Neha Agarwal, Dublin City University

14. Impact of Plasma Parameters on Plasma Enhanced Atomic Layer Deposition of Titanium Nitride

Darragh O'Neill, Dublin City University

15. Initial Characterisation and Processing of CuCrZr for Fusion Applications

Tom Hughes, The University of Manchester

16. In-Situ Process Monitoring of Additively Manufactured Ti-6-4

Alexander Sloane, The University of Sheffield

17. Line Edge Roughness: A Novel Approach for the Surface Roughness Measurement in Laser-Powder Bed Fusion Fabricated Parts

John Power, University College Dublin

18. Mechanics of Heterogeneous Case-Carburized Bearing Steels

Elif Sen, The University of Manchester

19. Modelling Non-Equilibrium Precipitation Kinetics in CuCrZr for Use in Plasma Facing Components

Samuel Engel, The University of Manchester

20. Processing History and Microstructural Characterisation of Titanium Alloys By In-Process Machining Force-Feedback

Dennis Premoli, The University of Sheffield

21. Silver Nano-Ink Generation via LASiS for Inkjet Printing of Temperature Sensor for Face Mask Application

Hasan Ayub, Dublin City University

**22.** The Computational & Physical Modelling of Powder Flow in Additive Manufacturing Andrew Burgess, Liverpool John Moores University

23. Through Process Modelling of Sustainable Aluminium

Vincent Kan, The University of Manchester

24. Towards a Circular Economy: A Case Study on Railway Track Sleepers

Jacob Whittle, The University of Sheffield

25. Using Life Cycle Assessment to Examine the Environmental Impact of Scrap Use in Steel Production

William Robertson, The University of Sheffield

#### **Poster Abstracts**

### Advancing Gear Oil Insights: Tribofilm and Subsurface Correlation Focusing on Ashless Versus Organometallic Chemistries

Ashutosh Gupta, The University of Manchester, ashutosh.gupta@postgrad.manchester.ac.uk Professor Allan Matthews, The University of Manchester & Ieuan Thomas, BP

The goal of the energy transformation is to eliminate energy-related CO2 emissions. If the world wants to accomplish the agreed-upon climate change targets, it must rapidly shift away from the use of fossil fuels and toward cleaner, renewable energy sources. Wind turbines have been rapidly developed and deployed around the world in response to the growing need for environmentally sustainable global power. The supporting bearing assemblies that allow for smooth, continuous operation and power generation fail considerably before their specified duration, which is a well-known problem with geared wind turbine drivetrains. Bearing failures are more prominent in the case of the wind turbine and in this study we have particularly focused on the hardened AISI 52100 steel used as a bearing material. The most important factor is the use of gear oils, which are specifically designed for lubrication and can reduce friction and heat generation while focusing on gear performance. In this research, three industrial-based gear oils will be examined to determine their suitability for various loading circumstances. The high-level goal of this project is to mitigate the problems related to breakdown time in wind turbines by considering the important tribological techniques.

### Assess Hydrogen Embrittlement Behaviour by Investigating the Impact of Different Electrochemical Charging Levels Through the Bulk Steel Specimen

Mehreen Kainat Khan, The University of Manchester, mehreen.khan-4@postgrad.manchester.ac.uk Dr Brian Connolly, The University of Manchester, Dr Phil Dent, Element Materials Technologies Ltd

The general consensus of this project is to tackle the critical issues surrounding hydrogen embrittlement. This is achieved by determining the behaviour and variation of hydrogen interaction with bulk steel material whereby hydrogen is trapped to molecular surfaces via adsorption. The pipeline steels are subjected to extensive cutting, polishing and grounding processes to ensure specimens are compatible with testing methods as discs. Thus, electrochemical charging is conducted at different charging levels and duration to introduce hydrogen into the metallic lattice structure; the data is collated and compared with electrochemical charging using hydrogen chloride (HCI) and hydrogen sulphide (H\_2 S) as an aqueous solution. This enables the metallography of steel specimens to be observed such that the physical structure and metallic components are discussed. Differences in diffusing the hydrogen solution at various electrochemical charging levels through the bulk material is examined via the Thermal Desorption Spectroscopy (TDS) technique; the desorption rate of atoms trapped within the lattice while heating the specimen at a specific rate is defined. The TDS method is considered a better alternative to the hydrogen permeation method due to the hydrogen desorption flux in a controlled temperature condition and indicates if hydrogen is trapped efficiently. Subsequently, the melt extraction provides accurate measurement of the hydrogen content. This may lead to further investigation into pursuing comparison of data obtained with gaseous electrochemical charging.

### Assessment of Local Ordering in the NiCoCr Ternary Alloy Down to Low Temperature via Total Scattering Analysis

Benjamin Jolly, The University of Sheffield, bejolly1@sheffield.ac.uk Dr Lewis Owen, The University of Sheffield

The following project aims to assess the impact of local ordering behaviour on the mechanical and compositional properties of a NiCoCr ternary alloy down to low temperature. Through the combined use of Bragg and Total Structure diffraction analyses, a large box modelling approach will investigate the short-range order of NiCoCr when cooled from ambient temperature to absolute zero, and the effect that this is likely to have on the local solid solution stability of the alloy. Data for this experiment has been provided by the Polaris detector of the ISIS Muon and Neutron Source; a comparative dataset will be produced in-house and evaluated through the use of SEM and EDX characterisation techniques. Simultaneously, the project will seek to evaluate the feasibility of applying equivalent evaluation techniques to more compositionally complex High Entropy Alloys (HEAs), an emerging class of materials ear-marked for use in the nuclear sector.

#### Characterisation and Thermodynamic Modelling of Mg-Zn-Gd-Zr Variant Alloys

Sian Odell, The University of Manchester, sian.odell@postgrad.manchester.ac.uk

Professor Joe Robson, The University of Manchester & Matt Murphy, Luxfer MEL Technologies

The majority of commercial magnesium alloys are grain refined by the addition of zirconium with the exception of magnesium-aluminium alloys. In this case the aluminium prevents the grain refining effect of the zirconium by the formation of an intermetallic compound. The interaction between other alloying elements and the refining zirconium is of interest in the development of magnesium alloys. Knowledge and understanding of the phases formed and the effect these have on the mechanical properties and corrosion resistance of the alloy created can be utilised in the development of new production alloys. Previous studies on the Mg-Zn-Zr system show that both the mechanical properties and grain refining effect are significantly affected by different compositions and the various compounds that can form as a result of the interaction between Zn and Zr during solidification or heat treatment. Further similar studies must be done to assess the interactions between Zr and other alloying elements in magnesium alloys and the effect these have on the properties. An experimental study will be carried out on three different compositions of the Mg-Zn-Gd-Zr alloy system, varying only the weight percentage of gadolinium. These alloys will be studied in both the as cast and heat-treated states with the precipitation of an LPSO phase being of high interest. The study shall include microscopy, microanalysis and mechanical testing. The results will be compared to various thermodynamic models of the same alloy compositions.

#### Creation of Digital Fingerprints from Machining Force Feedback Data

Joshua Taylor, The University of Sheffield, jtaylor25@sheffield.ac.uk
Professor Martin Jackson, The University of Sheffield & Rachid Masoub, Seco Tools AB

Titanium alloys are widely used in the medical and aeronautical industries due to their high strength to weight ratio. However, these components must undergo strict testing before being put into service, which is often time consuming, expensive, and destructive to the component. Digital fingerprints are being increasingly used in material and machining science to develop digital twins – virtualisations of real systems that can predict real world outcomes. Using machining force feedback, digital fingerprints were generated which can be used to infer information about the machine surface. The effect of two

different machining inserts (tungsten carbide and polycrystalline diamond) on the quality of the digital fingerprint produced is explored for five different titanium alloys. Results show that inserts that result in higher machining force, and therefore a higher noise to signal ratio, give better resolution digital fingerprints than the contrary.

# Development and Characterization of Calcium Phosphates Coating Layers on Magnesium Substrates for Control the Degradation Rate and Enhance the Bone Repair for Potential Orthopaedic Implantation Applications

Tina Sadat Hashemi, Dublin City University, tina.hashemi2@mail.dcu.ie Professor Nicholas Dunne. Dr Tanya Levingstone, Dublin City University.

Bone repair materials are rapidly becoming a hot topic in the field of biomedical materials due to being an important means of repairing human bony deficiencies and replacing hard tissue. Metallic implants are considered an excellent choice for bone fracture due to their high mechanical strength, high fracture toughness, corrosion resistance and biocompatibility during the bone healing period. Although surgeons rely on titanium or stainless-steel implants which are non-resorbable it highlights the need for second surgery to remove the implants. Magnesium and its alloys have been identified as promising bone implant materials owing to their good biocompatibility, osteoconductivity, natural ability to biodegrade in the body, and mechanical properties. Medical magnesium implant implants eliminate the need for a second surgery and as a result, it reduces healing time, risk of infection, pain, and the cost significantly. However, too fast a degradation rate in a physiological environment limits their clinical use in bone repair applications. Surface coating is one of the considerable solutions that has been used in this study. The bioactive calcium phosphate (Ca-P) is one of the most efficient and cost-effective routes to reduce the degradation rate of Magnesium and improve corrosion resistance while maintaining biocompatibility. In this study, octacalcium phosphate (OCP) coatings have been used as a means to control these corrosion rates. The magnesium specimens have been coated using an immersion technique. Within this investigation, the immersion technique was utilised as it is relatively inexpensive and scalable at an industry-level to produce an OCP coating on Mg-based medical implants. Coatings were characterised using energy dispersive spectroscopy (EDS), and scanning electron microscopy (SEM). The coating composition and crystallinity have also been determined using FTIR spectroscopy and XRD. Prior to the coating process, pre-treatment of the magnesium specimens was optimised to achieve the desired surface roughness. To optimise the adhesive strength of the coating to the surface of the magnesium specimen and the coating thickness - the effect of the digestion time and immersion cycle number were investigated. The adhesive strength was investigated using a tensile test method that was in accordance with ISO 13779-4. The thickness and surface morphology of the coating was determined using optical microscopy and SEM. The study results will determine the relationship between digestion time and immersion cycle number on the OCP coating thickness and the adhesive bond strength and the optimal coating parameter will be defined as a consequence. Next steps will focus on investigating the in vitro degradation of Mg substrate and the static mechanical properties as a function of degradation state will be determined.

#### Development of New Beta-Titanium Alloys for Additive Manufacturing of Biomedical Implants

Theo Mossop, University College Dublin, theo.mossop@ucdconnect.ie Dr Mert Celikin, University College Dublin & Dr David Heard, Stryker

Biomedical implants are a particularly suitable application for metal additive manufacturing (AM) technology where more complex geometries can be produced in comparison to traditional routes. However, most common  $\alpha$  /  $\beta$  titanium (Ti) alloys such as Ti-6Al-4V often suffer from reduced fatigue performance and notch-sensitivity due to steep heating and rapid cooling conditions of AM which limits the commercial use of this technology. Therefore, the need for developing novel Ti-based alloys more suitable for AM processing is clear. A new class of biocompatible  $\beta$ -Ti alloys based on the Ti-Nb system show promise for improved mechanical properties and ease-of-processing. In this work, two compositions of metastable  $\beta$ -Ti alloys, Ti-25Nb and Ti-20Nb-10Ta (wt%) with very similar  $\beta$ -transus temperatures are manufactured using both wedge-casting (slow cooling) and laser-remelting (rapid cooling). The effects of thermal gradient and solidification rate for both processes on microstructural evolution are investigated using electron microscopy and X-ray diffraction (XRD). The comparison of microstructural features between wedge-casting and laser-remelting will shed light into development of novel  $\beta$ -Ti alloys for biomedical applications.

#### **Effect of Heat Treatment on the Performance of Nitinol Wires for Actuators**

Josephine Ryan Murphy, Dublin City University, josephine.ryanmurphy2@dcu.mail.ie Professor Dermot Brabazon, Dublin City University & Michael O Donnell, FW Metals

In this study the effect of heat treatment on the performance of nitinol wires for actuators was investigated. In order to create a shape memory effect within the material, the wire samples are first formed into a spring shape, heated to an ageing heat treatment temperature and then quenched. For this study, samples of nitinol wires at austenite finish temperatures 0, 14, and 25°C provided by Fort Wayne metals were heat treated at 350, 400, and 450°C for 30, 60, and 90 minutes. These heat treatments were used to train the shape memory of the wire. These samples were then tested using an in-house designed and built wire actuator testing rig at DCU. For testing, a bias load is attached to the wire which pulls the wire straight. On application of an electric current across the wire, the wire heats above the phase change temperature and the wire returns to its original spring shape. The rig includes a thermal imaging camera that measures the temperature of the wire, a displacement sensor that measures the displacement of the bias load due to the wire extension, and a load cell which measures the force on the wire during the phase change. A LabVIEW program was used to measure these responses as the current was applied and removed. The results were used to determine the optimum heat treatment parameters and austenite finish temperature for the actuator response in terms of displacement, actuation time, and phase change temperature.

#### **Environmental Impacts of Alternative Blast Furnace Ironmaking Materials**

Siti Nurlisa Ahmad, The University of Sheffield, sahmad3@sheffield.ac.uk Dr Richard Thackray, The University of Sheffield & Peter Warren, British Steel

Steelmaking is a key industrial sector and has benefited modern society in terms of economics and global growth. Global steel production has significantly increased from 800 to 1900 million tons from 1990 to 2020. In 2020, the steel industry produced 2.6 billion tons of direct CO2 emissions, which accounted for 7-9% global anthropogenic CO2 emissions. Higher CO2 emissions are due to coal used

as fossil fuels. Coal contributes to ~ 74% energy inputs and is very cheap thus making the material a competitive choice. There is an increased pressure following the Paris Agreement to explore greener ways in steelmaking to achieve net carbon zero by year 2050. The main aim of this mini project is to assess the suitability of alternatives to fossil fuel (e.g., sub coal) as raw materials in ironmaking by using life cycle assessment (LCA) method. The second aim is to evaluate the suitability of various zinc recovery processes using an LCA. Familiarisation with the methodology and software used in conducting an LCA will also be a key focus of this mini project. The outcomes and training gained from the mini project will be used as a basis to meet some of the initial aims of the wider EngD project.

#### **Estimation of Fracture Toughness for Ferritic Steels in the Transition Range**

Kamila Nowosad, The University of Sheffield, kknowosad@sheffield.ac.uk Professor Dan Cogswell, The University of Sheffield & Andy Barton, Element Materials Technologies

Steels with the body-centred cubic lattice structure exhibit a ductile-to-brittle transition during which the material capacity for plastic deformation largely decreases as the temperature is lowered. Due to intrinsic fracture toughness data scatter in the transition region various probabilistic approaches have been proposed to describe the relationship between the fracture toughness and temperature. Master curve methodology is a standardised (ASTM E1921), probabilistic method widely used to characterise ferritic steels in the transition range through the reference temperature parameter, TO. A better understanding of what constitutes a valid TO value is required to prevent excessive conservatism in component design while maintaining a low probability tolerance for brittle fracture. This work presents the result of an assessment of the reference temperature validation procedure provided in the ASTM E1921 standard. A review of the statistical methods, model inputs, and assumptions applied in the standard was conducted, and two datasets were analysed following the standard methodology. The literature and data analysis highlighted some drawbacks of the standard method to calculate TO such as invalidation of potentially useful data, prediction inaccuracy in the lower and upper transition regions, and the significant margin applied to account for the uncertainties. The following main areas were identified for consideration in future assessments to mitigate the limitations and improve the interpretation of available data: (1) calculation of the TO estimate error; (2) shape parameter optimisation; (3) development of summary statistics framework; (4) development of a model incorporating features based on the fracture surface examination results and load-displacement data.

# Experimental Analysis of R-Phase NiTi Tube Actuators Using Conductive/Convective Heating Stage Lehar Asip Khan, Dublin City University, leharasip.khan@dcu.ie Hasan Ayub, Corné Muilwijk, Inam Ul Ahad, Professor Dermot Brabazon, Dublin City University

In the last few decades, Nitiol (NiTi) actuators have created a massive impact at the commercial level due to their application in various engineering and medical fields. NiTi wires sheets and tube actuators are a useful resource for harvesting any form of heat energy available. In any actuation application, the rate of actuation and actuation force are important parameters that determine the feasibility of the actuator. Current ongoing research aims to critically investigate and develop NiTi R-phased and martensitic phased actuators using commercially available material. Prior heat treatment and shape setting will be performed on the available NiTi material in the research lab facility at Dublin City University. A design test rig will be built capable of providing conductive and convective heating for cyclic heating and cooling of material consequently producing actuation. Input parameters such as heat flux, convective flux, and actuator shape setting will be optimised while the output parameters such as rate of actuation and actuation force will be reported and optimised. In the later stages of the

investigations will be diverted towards the additive manufactured materials for a comparison of NiTi built by conventional methods and additive manufacturing. Criticality of the NiTi actuators is the rate of solid-solid phase transformation which is linked to the temperature distribution. Therefore, convective heat transfer correlations will be presented for an enormous range of input parameters.

#### **Finite Volume Simulation of Extrusion Processes**

Ali Shayegh, University College Dublin, ali.shayegh@ucdconnect.ie Dr Philip Cardiff, University College Dublin

Large plastic deformation is common in material processing. The better we understand the evolution of a material during a process, the faster we can cut lead times in the design stage, as well as tooling costs and machining downtime. Numerical approaches may be utilised to expand our knowledge of every stage of processes, and as a result, to facilitate decision-making for economical process optimization. When it comes to numerical simulation of deformation in solids, there are three general approaches: Eulerian, Lagragian, and Arbitrary Eulerian-Lagragian (ALE). Eulerian formulation refers to integrating of the governing equations over a fixed mesh which is the common approach in Computational Fluid Dynamics (CDF). In Lagrangian formulation, on the other hand, mesh is attached to the workpiece. ALE approach combines the two aforementioned approaches. In ALE approach, mesh and material motion are decoupled; while element distortion is minimum, outer nodes are attached to the boundary. In the present project, we will take the Eulerian approach, and implement the Levy-Mises flow rule to calculate viscosity, which subsequently is used in generalised Stokes' constitutive law, applied to a solid during an extrusion process. Finally, the method will be applied to a benchmark problem to see how the results compare.

#### Heat Treatment of Nitinol Manufactured via L-PBF for Biomedical Applications

Neha Agarwal, Dublin City University, neha.agarwal2@mail.dcu.ie Professor Dermot Brabazon, Dublin City University & Michael O Donnell, FW Metals

Bespoke stents are the direction in which the medical field is advancing due to the patient specific requirements of each person's anatomy. To fulfil these needs, new technologies like additive manufacturing combined with the super-elastic property of nitinol can be taken advantage of. In this work, laser powder bed fusion (L-PBF) was used to print 5 by 5 by 5 mm cuboid samples with different process parameters (laser power, scan speed and hatch spacing). The samples were post-process heat treatment using three different temperatures (400, 500 and 600 °C) and ageing times (30, 60 and 90 min) according to a 3^2 design of experiments. The produced sample microstructures were analysed using Scanning Electron Microscopy. Sample crystal structure and elemental analysis were studied using X-Ray Diffraction and Electron Dispersive X-Ray techniques. Further work will include compression, hardness, and DSC for phase transformation analysis. The results from this study will enable determination if the L-PBF process can be used to produce parts with the physical and chemical properties required for biomedical applications.

#### Impact of Plasma Parameters on Plasma Enhanced Atomic Layer Deposition of Titanium Nitride

Darragh O'Neill, Dublin City University, darragh.oneill86@mail.dcu.ie Dr Deborah O Connell, Dublin City University & Rodger Nagle, Intel

Atomic layer deposition (ALD) is an advanced thin film deposition technique. Based on self-limiting, half-cycle reactions it produces conformal, thin films. Plasma enhanced ALD (PE-ALD) replaces the coreactants vapour pulse step of thermal ALD with a plasma pulse step. The reaction which occurs at the plasma-surface interface is critical for film growth. In this project, the impact of plasma parameters such as plasma power, pressure and gas flow will be investigated. This will be conducted by the analysis of the plasma through use of Optical Emission Spectroscopy (OES) during the deposition of a titanium nitride (TiN) film. The resulting chemical and structural properties of the TiN film will be analysed using X-Ray Photoelectron Spectroscopy (XPS).

#### **Initial Characterisation and Processing of CuCrZr for Fusion Applications**

Tom Hughes, The University of Manchester, thomas.hughes-7@postgrad.manchester.ac.uk Dr Ed Pickering, The University of Manchester & Dr Allan Harte, UK Atomic Energy Authority

This PhD will aim to provide some insight into how materials can be tested in a (mostly) realistic environment; the material chosen for this project is CuCrZr. CuCrZr is a prime candidate for the divertor and heat exchanger parts of the ITER, DEMO and potentially STEP nuclear fusion reactors. The divertor undergoes some of the largest heat fluxes of any part in the reactor; and due to CuCrZr's high creep resistance and thermal conductivity it will be very useful as a heat exchanger, as well as having some resistance to the hostile reactor conditions. However, to begin analysing how CuCrZr reacts under reactor conditions, it will be useful to gather a solid understanding and background for the alloy. This mini project will involve testing and analysing CuCrZr, provided by the UKAEA. Initial characterisation of CuCrZr should be a simple process, mainly involving sectioning the UKAEA-provided sample material and using a variety of techniques to quantify and analyse it. For example, optical microscopy, SEM and hardness testing. This should give an adequate insight into the material microstructure, composition, and properties. Hardness testing will be especially useful to compare the embrittling effects of radiation damage. The idea for this project, post initial characterisation, will be to then use CuCrZr samples in the in-situ testing rigs, without irradiation. A useful prospect for two reasons; firstly, allowing the student to get used to the preparation process and test rigs; and secondly allowing a useful comparison to the radiation testing that will come later down the line. It is worth noting that in fusion reactors there is a large amount of neutron radiation, but due to lack of neutron sources comparable to that of a reactor, this PhD will use proton radiation on thin samples. Thin samples predominantly because protons have lower penetration than neutrons.

#### In-Situ Process Monitoring of Additively Manufactured Ti-6-4

Alexander Sloane, The University of Sheffield, asloane1@sheffield.ac.uk Professor Iain Todd, The University of Sheffield & Lukas Jiranek, Boeing

The growing field of metallic Additive Manufacturing (AM) presents a great opportunity for various industries to rapidly produce complex parts, eliminating traditional needs for expensive tooling and, in many cases, multi-part assemblies. However, metallic AM techniques remain hindered by issues with part quality, predictability, and reproducibility. Parts created using Laser Powder Bed Fusion (L-PBF) regularly contain porosity defects. The two most common defects are: Lack of Fusion pores,

where the powder particles did not fuse together due to a lack of thermal energy; and Keyhole pores, where powder particles evaporate and eject molten material under recoil pressure, due to an excess of thermal energy. This current work retrospectively explores the conditions under which each type of pore defect occurs in the L-PBF AM of Titanium-6-4, with future ambitions to develop this knowledge into in-situ control systems, with the ability to predict the production of each defect type during the manufacturing process. Three machine parameters were tested: laser speed, laser power, and hatch spacing. Several hundred samples, each with a unique combination of these parameters, were manufactured and analysed. The quantity and type of resulting pores were measured, and compared to pyrometric data recorded during the build, calculated values of thermal energy input, and numerical predictions of melt pool volumes, for each sample. Correlations between these four data sets were analysed, in an attempt to better understand the conditions likely to impart either too much or too little thermal energy into the Ti-6-4 powder.

### Line Edge Roughness: A Novel Approach for the Surface Roughness Measurement in Laser-Powder Bed Fusion Fabricated Parts

John Power, University College Dublin, john.power1@ucdconnect.ie
Mark Hartnett, IMR & Professor Denis P. Dowling, University College Dublin

Additive manufacturing (AM) is widely used in the fabrication of metallic parts for use both in the medical device and aerospace sectors. One key characteristic used to measure the quality of an AM produced part, is the roughness of the printed alloy surface. Conventional methods for the measurement of roughness, such as the stylus and optical profilometry, have considerable difficulty in measuring features on difficult to access geometric features, such as overhangs. In this work, a Line Edge Roughness (LER) approach has been developed in order to provide a quantitative assessment of the printed AM part roughness. These measurements are based on data obtained from cross section optical microscopy images of overhang features. These features were obtained for Ti-6Al-4V parts, printed using the laser powder bed fusion technique. The LER technique quantitatively defines the roughness of an edge, based on an analysis of ImageJ software data, obtained from cross section microscopy images of that edge. The roughness measurements are obtained based on the deviation from an ideal shape. The titanium alloy test samples were printed with varying laser powers to investigate the effect of laser energy on the roughness of the resulting overhang features. At higher laser powers an increase in the roughness of the part was observed. This increase is due to overheating of the melt pool formed by the laser, as it interacts with the powder particles. This overheating is associated with the comparatively lower ability of the powder particles, directly underneath the overhang to remove heat, due to their lower thermal conductivity, in comparison with that obtained for the solid alloy structure. In order to obtain a quantitative assessment of the performance of the LER technique, comparative roughness measurements were obtained using optical profilometry for 'exposed' printed overhang structures.

#### **Mechanics of Heterogeneous Case-Carburized Bearing Steels**

Elif Sen, The University of Manchester, elif.sen@postgrad.manchester.ac.uk

Dr Enrique Jimenez-Melero, The University of Manchester & Mohan Paladugu, Timken

Bearings are precision components used for load transfer and motion in various equipment and industrial machinery. Their primary role is to provide the smoothest rotation of two rotating parts with the least possible friction. Another role is to protect the part that supports the rotation and maintain the proper position for the rotating shaft. These industry-wide components are also referred to as the

"industry's bread and butter", as they are found in nearly everything from household appliances to gearboxes and conveyor systems in electric motors. During operation, bearings are subjected to severe shock loads hence they are expected to have high resistance to impact and high rigidity. Therefore, hardening processes are widely used to obtain high surface hardness and wear resistance from these engineering components. The method used to harden the surfaces of low carbon steel is called carburising. Carburised steel microstructures are multiphase structures and include martensite, retained austenite, and carbides. However, depending on the carburisation parameters used, there is usually a change in the number of near-surface carbides, grain size, carbon content, volume ratio, and local environment of metastable austenite. Therefore, there is an industrial need to prove the mechanics of carburised bearing steels through their thicknesses. Studies are desirable to correlate the local microstructure and production of bearing steels with their mechanical behaviour. Hence, the characterisation of the as-received case-carburised steels will be compared with the standard throughhardened QT microstructures during the project. Also, it is necessary to evaluate the impact of non-QT bainitic/martensitic microstructures, produced by either austempering or quenching and partitioning, on the bearing mechanics.

# Modelling Non-Equilibrium Precipitation Kinetics in CuCrZr for Use in Plasma Facing Components Samuel Engel, The University of Manchester, samuel.engel@postgrad.manchester.ac.uk Professor João Quinta da Fonseca & Dr Pratheek Shanthraj, The University of Manchester

The advancement of nuclear fusion is significantly limited by the available materials that can withstand the extreme environment experienced by plasma-facing components. For research to continue efficiently, modelling approaches are required in order to predict the evolution of these materials under intense conditions, with focus on developing models for microstructural characteristics. This study presents a model for precipitation kinetics with curing time in CuCrZr alloys across various ageing treatments. A multi-class KampmannWagner Numerical modelling framework is used to describe the evolution of the precipitate size distribution, which has been calibrated with time dependant precipitation data from literature and further tested against experimental data in order to establish the model's temperature dependence. The predicted precipitation kinetics accurately reproduce the long-term coarsening behaviour of coherent FCC precipitates, which was utilised to infer how the alloy microstructure evolves when at a working temperature relevant to fusion materials.

### Processing History and Microstructural Characterisation of Titanium Alloys by In-Process Machining Force-Feedback

Dennis Premoli, The University of Sheffield, dpremoli1@sheffield.ac.uk Professor Martin Jackson, The University of Sheffield & Kyle Marshall, Rolls-Royce

Machining trials were run, to better understand and refine the use of digital fingerprints as a novel characterisation tool. These focused on 4 different alloys: Ti-6Al-4V (sub and super-transus in nature, obtained through Field Assisted Sintering Technology (FAST), Ti-17, Ti-5Al-5Mo-5V-3Cr, and Ti-10V-2Fe-3Al. The forces experienced by various cutting tools and inserts were recorded through a dynamometer and the data obtained was analysed and converted into polar force scatterplots. New software was created to streamline the data-acquisition to image-generation process, resulting in increased data analysis time. In-process machining force-feedback successfully highlighted microstructural features and residual stresses stemming from the materials' varying processing

histories. Further work remains to validate the microstructural results found, through a secondary means of characterisation such as Electron Backscattered Diffraction.

### Silver Nano-Ink Generation via LASiS for Inkjet Printing of Temperature Sensor for Face Mask Application

Hasan Ayub, Dublin City University, hasan.ayub@dcu.ie

Ronan McCann, Terence Bowden, Lehar Asip Khan, Inam Ul Ahad, Karsten Fleischer & Professor Dermot Brabazon, Dublin City University

In this study, (Ag) silver nanoparticle (NP) colloids are produced using Laser Ablation Synthesis in Solution (LASiS) or Pulsed Laser Ablation in Liquid (PLAL) for ink generation. This technique resulted in a high yield form of the Nano colloid. Silver Nano colloid is used to produce silver Nano inks. The silver Nano ink or conductive ink has a substantial role in printable electronic devices such as temperature, pressure, and humidity sensors as well as in wearable sensors for health monitoring applications. The aim of current ongoing work is the generation of silver NP ink with LASiS technique and printing it over the flexible substrate using aerosol jet printing or FUJI diametric 3D printer. Further, characterisation of the printed ink tracks is performed which includes thermal and electrical conductivity, surface roughness and morphology. Moreover, the printed sensors combined with additive manufacturing of multi material leads to the prototype of smart face masks for health monitoring. The smart facemask comprises a sensor module mounted on it which contains the IC Board, health monitoring sensors and battery. The data acquisition received by the IC board is sent to the IoT (Internet of thing) platform. The IoT enables the live monitoring and storage of output data. The smart face mask can be utilised as a smart sports face mask for sports persons monitoring fitness and VO2 levels. Also, it is suitable for air filtration to observe the breathed air quality.

#### **Through Process Modelling of Sustainable Aluminium**

Vincent Kan, The University of Manchester, kwanhin.kan@postgrad.manchester.ac.uk Professor Joseph Robson, The University of Manchester & Mike Clinch, Innoval Ltd

Through process modelling (TPM) can assist in optimizing the thermomechanical processing of rolled aluminium plates and sheets by minimizing trial-and-error experiments. TPM can also accelerate the introduction of new alloys or alloys with high recycled content. A key component of a TPM for aluminium rolling is the prediction of the deformation and recrystallization behaviour. However, deformation and recrystallization are strongly affected by local heterogeneities in aluminium (e.g., second phase particles), especially for recycled alloys with high impurity content. To capture the effects of these heterogeneities, a full field crystal plasticity (CP) model has been used, enabling local strain distribution to be predicted. This model has been applied to particle containing alloys to study the effect of changing distribution of constituent particles. The predicted local strain distribution from the CP model will be used to initialize a full field recrystallization model. However, the disadvantage of full field modelling is the intense computational requirements, leading to long run-times which is undesirable in industry. To this end, a less computationally intensive semi-empirical model is envisaged.

#### Towards a Circular Economy: A Case Study on Railway Track Sleepers

Jacob Whittle, The University of Sheffield, jwwhittle1@sheffield.ac.uk Professor David Fletcher, The University of Sheffield & British Steel

Railway track infrastructure is principally constructed from rails, sleepers and various grades of ballast. Sleepers form a critical part of this infrastructure as they provide support for the rails above as well as preserve gauge, level and alignment of the track. As part of this the sleepers will transmit vertical, lateral and longitudinal forces from the rail to the ballast. Across the world there are approximately 3 billion railway sleepers in use, of which 95% are made of wood. However, in order to extend their life by several times these sleepers are coated in creosote, the use of which was banned in the UK and all EU member states from July 2021. This means that sleepers of alternative materials are suddenly more economically viable to infrastructure operators such as Network Rail and are actively being considered for use. However, there has been limited detailed or holistic research into the true-life cycle costs of different sleeper types; likely due to their limited use to-date when compared to wood as well as the reluctance to change existing infrastructure. This paper compares different sleeper materials on their performance, environmental and economic suitability for the role of a mainline railway sleeper. Given the current severely restricted use on wooden sleepers, this analysis focuses principally on the main alternatives by use of steel, concrete and composites.

### Using Life Cycle Assessment to Examine the Environmental Impact of Scrap Use in Steel

William Robertson, The University of Sheffield, wrobertson1@sheffield.ac.uk Dr Richard Thackray, The University of Sheffield & Dr Peter Hodgson, Tata Steel

Steel is primarily produced using the Blast Furnace / Basic Oxygen Furnace process. The amount of scrap that can be used in this process is limited to about 20%. The Electric Arc Furnace process allows for up to 100% recycled scrap content. A shift towards more production using the Electric Arc Furnace process could be an important step in reducing CO2 emissions. However, there are many factors besides the direct scrap use that could affect emissions and thus need to be investigated. This mini project aims to use life cycle thinking and relevant methodology to measure the environmental impact of (i) changes to the existing production routes of BF/BOF steel, and (ii) the use of scrap in the EAF process. These two case studies will provide a practical application for the Life Cycle Assessment process.

#### **Oral Presentation Abstracts**

#### 3D Printing of Continuous Stainless-Steel Fibre/Polymer Composites

Alison Clarke, University College Dublin, alison.clarke1@ucdconnect.ie Dr Andrew Dickson, Professor Denis P. Dowling, University College Dublin

This study investigates the fabrication of continuous 316L stainless steel fibre bundle (SSF) polymer composites using the Fused Filament Fabrication (FFF) technique. Fibres in the SSF have a diameter of 14 μm. This SSF was coated with a polylactic acid (PLA) polymer by co-extrusion, to form a filament. The resulting continuous PLA-SSF filaments have diameters of between 0.9-0.5 mm. The steel fibre reinforced filaments were used to print composite test samples by FFF, with the dimension of up to 3 x 15 x 170 mm. A particular focus of this research was the investigation of how the steel filament volume fraction in the resulting composite could be controlled in the range of 6 to 12 vol %. The samples exhibited a homogeneous distribution of steel filaments in the polymer matrix. To improve the volume fraction and the porosity of the structure, a number of alterations to the 3D printing methods were investigated. Parameters include layer height, path width, temperature and cooling. The samples exhibited a homogeneous distribution of steel filaments in the polymer matrix. The PLA-SSF composite samples are examined to evaluate their mechanical properties (tensile and interlaminar shear strengths), porosity (CT scans and cross-section studies), as well as morphology (microscopy and SEM examination). The ability of the FFF technique to fabricate PLA polymer-SSF composite structures exhibiting relatively low porosities (6 %), was successfully demonstrated. Based on mechanical testing studies it was demonstrated that SSF reinforcement of the PLA increased interlaminar shear strengths by 544%. In order to assess the performance of the steel reinforced composite, a comparison was made with carbon fibre reinforced PLA polymer composites. Compared with the carbon fibre composite the interlaminar shear strength (ILSS) of the steel composite was significantly higher, however, the volume fraction of the fibre needs to be considered. There is considerable potential for printed steel composites for individualised conductive composite applications. The mechanical strength achieved is higher than for any 3D printed composite continuous metal filament reported to date.

### Additive Manufacturing for the Development of Microneedle Arrays as Minimally Invasive Drug Delivery Systems

Nikoletta Sargioti, Dublin City University, nikoletta.sargioti2@mail.dcu.ie Dr Nicholas Dunne, Dublin City University & Helen McCarthy, pHion

Current drug delivery systems (e.g., topical creams, transdermal patches etc.) have associated limitations including pain and poor administration of small and large drug molecules [1]. A painless micro-sized device capable of achieving easy and efficient drug delivery, with no side effects is required [2]. Additive manufactured microneedles (MNs) have been considered as an optimal and cost-effective innovative platform. This research aims to develop a 3D–printed stainless steel (316L) MN array with optimal mechanical/biological properties for disease management and treatment. Initially, a parametric study was conducted using a Design of Experiment (DoE) approach to optimise and validate the printing parameters followed by experimental investigations of the functional properties of MN arrays (e.g., penetration and drug elution studies).

### An Investigation into the Effect of Microtextured Regions on the Fatigue Properties on Forged Titanium

Patrick Curran, The University of Manchester, patrick.curran@postgrad.manchester.ac.uk Professor Joao Quinta da Fonseca, Dr Pratheek Shanthraj, Professor Philip Prangnell, The University of Manchester & Benjamin Dodd, Airbus

Large industrial forgings of titanium alloy Ti64, are used in modern airframes. These components are used in the  $\beta$ -annealed condition, which produces a microstructure made up of large lamellar grains, with coarse laths, a consequence of the slow cooling rates in large forgings. When the material is cyclically loaded, strain and stresses will localise within these coarse grains, which could lead to fatigue crack initiation. In this project in-situ high resolution digital image correlation (HRDIC) of monotonic and cyclic loading were carried out. The results were compared to computational modelling, using the crystal plasticity modelling framework DAMASK. Simulations were made using different constitutive laws, with and without back-stresses, to predict how the strain localises. Both experiments and simulations showed that strain localised in grains that were well-aligned for prismatic and basal slip. Although using the constitutive behaviour with back-stresses provides better agreement at the macroscale, it does not significantly change the strain localisation at the microstructural scale. The implications of these results for modelling the strain localisation in  $\beta$ -annealed Ti64 microstructures is discussed.

### Anti-Ice Fouling Surfaces by Fabrication Superficial Structures on Aluminium Alloys by Laser Machining

Abhijit Suhas Cholkar, Dublin City University, abhijit.cholkar2@mail.dcu.ie Suman Chatterjee, Dr David Kinahan, Professor Dermot Brabazon, Dublin City University

Ice or frost production and deposition on the surface is known as icing. Increased energy consumption, decreased energy conversion efficiency, mechanical or electrical malfunctions, and safety issues can all develop as a result of these problems. To avoid this, surface modification is necessary. Various technologies, such as anti-icing surface coatings and chemical surface treatments, have been developed over the years to reduce ice formation and adhesion to substrates in contact with fluids present under freezing temperatures. One route toward the generation of anti-icing surfaces is through laser surface processing. Laser micro/nano structuring of surfaces has advanced greatly in recent years due to advancements in laser source technology and reduction in capital costs for ultrafast femtosecond pulsed machining lasers. A novel process of laser micro/nano structuring of surfaces has been proposed aiming to produce anti icing surfaces. In this research we demonstrate the production of anti-icing surfaces using a femtosecond laser micro and/or nano structuring on the aluminium alloy substrate which is used in the aerospace application. The experiment is designed to get the most optimised anti icing surface on the aluminium. The laser parameters such as pulse energy, repetition rate and scanning velocity are varied for producing microstructures on the aluminium surface. To test for the anti-icing properties wetting properties are defined by contact angle measurements and the surface morphology is characterised using the optical profilometry. Various functional properties such as hydrophobicity and surface roughness are examined.

### Characterisation of Zirconium Alloys with Copper and Vanadium Additions for Nuclear Fuel Assembly Materials

Callum Andrew, The University of Manchester, callum.andrew@postgrad.manchester.ac.uk

Dr Philipp Frankel, The University of Manchester & Mangus Limback, Westinghouse Electric Sweden

Zirconium alloys are used as nuclear fuel assembly material in water-moderated nuclear reactors, primarily due to their low neutron cross-sections. One limitation of zirconium alloys is that the hexagonal crystal structure of α-Zirconium and strong texturing from manufacture lead to macroscopic irradiation-included growth (IIG). Developing alloys that show improved resistance to IIG can improve in-reactor efficiency – a critical aim in extending fuel lifespan, alongside reducing waste. Recently, Westinghouse Electric AB developed zirconium alloys with copper and vanadium additions, which showed improved IIG performance compared to previous cladding generations. Currently, there are gaps in the mechanistic understanding of the roles that copper, and vanadium additions play in zirconium alloys, and this PhD project seeks to improve the mechanistic understanding of these elements during irradiation, focusing on IIG. Unique alloy compositions are being studied in this project, the W10 (Zr-1Nb-0.3Sn-0.2V-0.05Fe) and W13 (Zr-1Nb-0.3Sn-0.2Cu-0.05Fe) alloys developed by Westinghouse, which were neutron irradiated in the BOR-60 research reactor. Baseline characterisation of the alloys is needed, to understand how copper and vanadium influence alloy microstructure, and to act as a reference for microstructural evolution during irradiation. The findings of the baseline characterisation of the W10 and W13 alloys to date are presented in this presentation.

#### Computational Study of Microstructurally Short Crack Propagation in AA7XXX alloys

Cameron Grant, The University of Manchester, cameron.grant-3@postgrad.manchester.ac.uk Dr Pratheek Shanthraj, The University of Manchester & Dr Christian Engel, Airbus

Environmentally assisted cracking (EAC) in humid air is a type of degradation behaviour which can lead to a severe decrease in the mechanical performance of 7XXX series aluminium alloys. These new generations of 7XXX Al alloys, such as AA7085 and AA7449, are now hot topics in the scientific literature because of their comparatively poor EAC performance. Alloys such as AA7050 perform significantly better in humid environments. Existing scientific literature has not yet thoroughly investigated how the microstructure of these alloys impacts the growth and lifespan of microstructurally short cracks. 3D crystal plasticity simulations have been used to investigate the extent to which microstructural features can impede and resist short crack growth. Specifically, by considering highly misaligned grains and recrystallised grains, it is possible to quantify the extent to which short crack propagation can be impeded by microstructural features. This has allowed the comparison of strain energy release rate values in the case of unimpeded crack growth vs impeded crack growth. Such comparisons provide excellent insight into the nature of microstructurally short crack propagation.

#### Coupling Component Diffusion with the Precipitation Kinetics of Ni-Based Superalloys

Sakina Rehman, The University of Manchester, sakina.rehman@postgrad.manchester.ac.uk Professor Joao Quinta da Fonseca, The University of Manchester & Christos Argyrakis, Rolls-Royce, Derby

When exposed to high-temperatures and corrosive reagents, turbine-disc Ni-based superalloys form protective oxide layers along the surface of the superalloy. Subsurface is a region depleted in the gamma' precipitate phase as a result of the diffusion of solute species from the gamma' precipitates

to the surface oxide. As these superalloys are precipitate strengthened by the dispersion of coherent gamma' precipitates, this depletion leads to a detrimental effect on the mechanical properties. A mean field model has been developed to model the gamma' precipitate depletion zone in RR1000, a commonly used Ni-based turbine-disc superalloy. Initial particle size distributions (PSD) are divided into a series of discrete size classes, corresponding to the equilibrium phase fraction of gamma'. The model consists of a multicomponent diffusion driven solute-rate law, which calculates the dissolution rate of each discrete particle size class. This is based upon CALPHAD obtained energy and mobility expressions of the solutes contained within the oxide. Three test cases were investigated: (1) Model calibration, i.e. the model is validated against existing precipitate depletion zone kinetics for RR1000 (2) the effect of temperature on the PSD, specifically as the gamma' solvus temperature (~1100C) is reached (3) the effect of oxygen partial pressure (ppO2) on the PSD i.e. a larger ppO2 leads to an increased oxide growth rate, hence a higher outwards flux of solute (4) the effect of altering alloy composition on the PSD. Further work would involve coupling this model to a crystal plasticity model, to model the competition between oxide wedge protrusion stresses against precipitate dissolution stress relaxation and to also spatially resolve the precipitates in a phase field model.

#### **Design of HEA Hardmetals for Tooling Applications**

Joshua Berry, The University of Sheffield, jberry1@sheffield.ac.uk
Dr Kathy Christofidou, The University of Sheffield & Dan Johns, Oerlikon

High entropy alloys differ from conventional alloys, in that they consist of multiple principal components. Resulting in a vast number of possible compositions, each with potentially advantageous combinations of mechanical and structural properties, that can be easily adapted to suit the application. Thus, high entropy alloys present an opportunity for the design and development of new wear resistant hard metals, to replace the conventional WC-Co cemented carbides, used in demanding metal forming applications. However, the vast compositional space occupied by high entropy alloys results in unguided experimental searches being unfeasible. Here, a random forest machine learning architecture, in conjunction with the CALPHAD method, is trained to select a sample of high entropy alloy compositions, for experimental testing. The random forest models were trained from experimental, high entropy alloy, thermal and mechanical property databases. Prediction accuracies of (78.7±4.8) % and (82.1±1.9) % for phase formation and (66.1±9.5) HV for alloy hardness were achieved from the random forest models. Nine of the hardest high entropy alloy compositions, predicted to form FCC solid solution phases by the machine learning models, were selected. Experimental assessment of these selected alloys will provide information on their suitability for WC-Co replacement, while simultaneously enabling verification of the machine learning methodology and providing further data for future model development.

#### Development of Novel Numerical Methods for Metal Forming of High-Strength Steels

Federico Mazzanti, University College Dublin, federico.mazzanti@ucdconnect.ie Professor Denis Dowling, University College Dublin & Veerle Van Wassenhove, Bekaert

Material processing techniques, such as drawing and rolling, are used to manufacture metal rods and wires, which could be used for a variety of applications, for example, as reinforcements for mines, tunnels and roads, or in the automotive industry, among many others. However, in order to produce high-strength wires or rods, the raw metal must go through a series of multiple passes, which must be specifically designed to achieve the desired geometry and properties. The design process could take even months or weeks and it would fully consist of trials and errors. Therefore, metallurgists and

engineers constantly incur an enormous optimisation problem. They might attempt to modify the tool design based on previous experience, but this is not an ideal approach to the problem. One of the most promising ways to solve this problem is to compute an efficient, accurate and robust roller design tool by simulating the processing route using the Finite Element or Finite Volume Methods. These methods could dramatically accelerate and cut down the costs of the industrial process. They could provide a significant reduction in error for different applications and predict final properties of complicated 3D geometries. This project focuses on simple linear elastic problems in an attempt to simulate them using a segregated and block-coupled Finite Volume Formulation. The accuracy of the solutions is also analysed in two different ways for multiple mesh sizes: a comparison between coarser and finer meshes; and the implementation of the Method of Manufactured Solution using a known trial function. The order of accuracy is then properly determined and benchmarked with results obtained in OpenFOAM using the solids4foam toolbox.

### Development of an Optical Fibre Mid-Wave Infrared Thermometer for Metal Machining Operations

Emilios Leonidas, The University of Sheffield, eleonidas1@sheffield.ac.uk

Dr Jon Wilmott & Dr Matthew Hobbs, The University of Sheffield, Dr Sabino Ayvar-Soberanis & Dr

Hatim Laalej, Advanced Manufacturing Research Centre, Rotherham, & Dr Stephen Fitzpatrick,

Advanced forming Research Centre, Paisley

During the machining process, substantial thermal loads are generated due to tribological factors and plastic deformation. The increase in temperature during the cutting process can lead to an accelerated tool wear, reducing the tool's lifespan; the degradation of the machining accuracy in the form of dimensional inaccuracies; thermally induced defects affecting the metallurgical properties of the machined component. Temperature is an important machining parameter; however, it is one of the most difficult parameters to monitor especially in high-speed milling application, this is due to the high rotational speeds of the cutting tool and the aggressive machining environments. In this study, a new fibre optic Infrared Radiation Thermometer (IRT) has been developed as the basis for temperature measurements during machining operations. The IRT is sensitive to wavelengths between 3 and 3.5 μm, which comprises an Indium Arsenide Antimony detector, a transimpedance amplifier and a sapphire fibre optic cable. A preliminary lab testing, using black-body approximation furnaces, of the proposed temperature measurement system showed that the thermometer is capable of measuring temperature between 200-1200°C with a maximum noise equivalent temperature resolution of 0.5°C at 200°C at an integration time of 1 ms. The proposed system has the potential to be embedded in a cutting tool to monitor the temperature at the tool-chip interface during cutting operations and to solve the problem of temperature measurements in a wide range of machining applications.

#### **Development of Advanced High Modulus Steels for Automotive Applications**

Sully Khan, The University of Sheffield, skhan31@sheffield.ac.uk
Professor Eric Palmiere & Professor Martin Jackson, The University of Sheffield, Dr Ralf Rablbauer,
Volkswagen, Wolsfburg

By introducing a new element or changing the weight percent (wt.%) of an element within steel, improvements can be observed in ultimate tensile strength, a key mechanical property in the automotive industry. Some examples which highlight the use of steels in a traditionally made automobile are car body panels, chassis, engines, and exhaust components. From these examples, it

can be determined that steel is an integral structural material and now has the potential to become lower in density whilst retaining/improving strength (commonly referred to as advanced high strength steels, AHSS). This is achieved by synthesis of metal matrix composites through introduction of ceramic particles such as titanium diboride (TiB2), niobium diboride (NbB2) and vanadium diboride (VB2) into steel matrix. Another aspect to consider when manufacturing steel is the thermomechanical processing route used for grain refinement, as this greatly affects microstructure and hence, mechanical properties. This project aims to conduct research and testing on steel composites via two routes, which are named 'vacuum-induction melting' (VIM) and 'field-assisted sintering technology' (FAST). VIM is the melting of a metal within a vacuum whilst utilising electric current whereas FAST uses a direct current (DC) coupled with compressive force to consolidate powders together. Both methods will allow the production of steel ingots with different compositions, which can then be put through hot rolling. From this, mechanical testing and microstructural analysis can be performed, and suitable steel-matrix composites will be finalised for production at an industrial scale. This project acknowledges Volkswagen as the industrial sponsor for this PhD.

#### Effect of Microstructure on the Localised Corrosion of 15-5PH Stainless Steel

Alyshia Keogh, The University of Manchester, alyshia.keogh@postgrad.manchester.ac.uk Alex Wilson, Dr Fabio Scenini, Professor Phil Prangnell, The University of Manchester

Maraging steels undergo a complicated heat treatment whereby they are solution treated to obtain a fully martensitic microstructure and then aged to produce finely dispersed strengthening precipitates that result in excellent mechanical properties including ultra-high strength and hardness whilst maintaining ductility. However, these steels can be susceptible to environmentally assisted cracking (EAC) in service and the mechanisms involved in EAC are not well understood. This project aims to enhance the understanding of EAC in maraging steels and evaluate the role that the microstructure plays on the corrosion behaviour. To achieve this, the evolution of the microstructure was assessed as a function of the secondary ageing treatment temperature to understand its role on localised corrosion. In the present study, maraging steels (mainly 15-5PH) with different ageing treatments were studied using potentiodynamic polarisation methods and atmospheric cracking tests. Initial results indicate that all the microstructures tested are susceptible to some form of localised corrosion. It is thought that the over-aged (higher temperature) microstructure is the most susceptible to localised corrosion but the most resistant to cracking whilst the under-aged (lower temperature) microstructure is the most resistant to localised corrosion but the most susceptible to cracking. The over-aged microstructure was found to contain a greater phase fraction of austenite compared to the underaged and peak-aged microstructures which is thought to contribute to its resistance to cracking. However, a more in-depth microstructural characterisation is required to establish the differences in the microstructures that are causing the difference in corrosion behaviour between the heat treatments. In addition, the materials response to hydrogen embrittlement and pitting initiation will also be investigated in future work with the overall intention to correlate microstructural features to the materials susceptibility to localised corrosion and hydrogen embrittlement.

### Influence of Solution Heat Treatment Temperature and Holding Time on the Microstructure, Texture, and Hardness of IN718 Produced by the L-PBF

Merve Nur Dogu, Dublin City University, mervenur.dogu@dcu.ie

Kemal Davut, Izmir Institute of Technology, Turkey; Muhannad Ahmed Obeidi & Professor Dermot Brabazon, Dublin City University; Mustafa Alp Yalcin, Metal Forming Center of Excellence, Atilim University, Ankara, Turkey; Hengfeng Gu, Thaddeus Song En Low & Jon Ginn, Ansys Inc., USA

Ni-based superalloys have been widely used for aerospace and industrial applications over the past four decades for their outstanding high-temperature mechanical properties. IN718, developed by the Nickel Corporation in the 1950s, possesses superior properties to many alternative alloys such as excellent oxidation and corrosion resistance, good weldability and high-temperature mechanical property stability up to 650 C. For this reason, IN718 is used in the aerospace industry, chemical and petrochemical industries and nuclear power systems. Additive manufacturing (AM) techniques provide significant advantages over conventional manufacturing techniques such as greater design freedom, near-net-shape fabrication, high material-use efficiency and alleviating the machining difficulty resulting from conventional manufacturing techniques. The laser-powder bed fusion (L-PBF) process is a metal AM technique that uses a focused laser beam to melt metal powder. Furthermore, the L-PBF process possesses a low buy-to-fly ratio, enabling the manufacturing of complex geometries in a single production step and often provides cost and time-saving advantages over conventional manufacturing. However, the high cooling rate of the L-PBF process causes rapid solidification leading to the formation of non-equilibrium phases such as Laves and carbides, inhibition of the precipitation strengthening phases, and microsegregation of the refractory elements such as Nb and Mo. Such cooling rates can also lead to high residual stresses which are undesirable. These can decrease mechanical performance. For this reason, post-heat treatments are often used as a common practice to dissolve detrimental phases (i.e., Laves), reduce possible residual stresses, and to optimise the microstructure and mechanical properties of the IN718 produced by the L-PBF. In this study, the influence of three different solution heat treatment temperatures (1050, 1150 and 1250 C) and holding times (15, 45 and 90 min) followed by furnace cooling (FC) under argon atmosphere on the recrystallization and grain growth behaviour of IN718 produced by the L-PBF was investigated. Microstructure and grain examination of the samples was performed using an optical microscope (OM), scanning electron microscope (SEM) and EBSD. Texture evolution of the samples was investigated using EBSD and microhardness values of the samples were measured by the Vickers microhardness test.

#### In Situ Characterisation of the Thermomechanical Deformation Behaviour of Powder Processed Ni-Based Superalloys

Frances Synnott, The University of Sheffield, fsynnott1@sheffield.ac.uk

Dr Kathy Christofidou, Dr Lewis Owen, Professor Martin Jackson, The University of Sheffield, Professor Howard Stone & Professor Nick Jones, University of Cambridge, Dr Paul Mignanelli & Dr Mark Hardy, Rolls Royce, Derby

Polycrystalline Ni-based superalloys are continuously evolving in order to enable improved properties and higher operating temperatures in critical applications in the aerospace industry. Compositional modifications are sought that can improve both the mechanical and environmental performance of new alloys. To understand the relative merits of Ti and Ta co-additions on the deformation of polycrystalline superalloys, three powder-processed alloys with varying Ti:Ta ratios were investigated

in situ under tensile loads in the temperature range  $600-800^{\circ}$ C using advanced synchrotron X-ray diffraction. The results enabled the quantification of the effect of the co-additions on the lattice misfit, elastic constants, and load partitioning between the  $\gamma$  and  $\gamma'$  phases as a function of composition and temperature, providing invaluable information on the deformation characteristics of the constituent phases. This work was supported by Rolls-Royce plc, SFI [18/EPSRC-CDT/3584] and the EPSRC [EP/S022635/1]. Data was collected at the Diamond Light Source [EE9270] and the ESRF [ME1344].

#### Measuring Image Quality of 3D X-Ray Computed Tomography

Jamie McGregor, The University of Manchester, jamie.mcgregor@postgrad.manchester.ac.uk Dr Tim Burnett, The University of Manchester & Dr Nick Bazin, AWE

Within X-ray computed tomography, gaining a final image result of sufficient clarity is vital to extracting trustworthy data. To quantify this clarity, there exists a series of image quality parameters that represent the different measurements within the tomogram. The contrast-to-noise ratio, signal-to-noise ratio, the optical transfer function and spatial resolution are prime factors to be investigated and can be related to the ease of both manual and automatic recognition of features. Image quality parameters can be measured directly from calibrated components with known constraints following standards defined through different recognised organisations. However, to measure the same values on objects of unknown architecture, such as an industrial or academic sample, advanced methods are required to locate regions of homogeneous and inhomogeneous material. Effort has been made to create a series of analysis techniques to fully understand a final image and to produce an image quality report. This data can be used with uncertainty declarations to gain confidence in results and to gain a greater understanding of the isolated features.

#### Methodologies Used in the European Countries for Critical Material Assessment

Ahmar Murtaza, Dublin City University, ahmar.murtaza@dcu.ie Sithara Sreenilayam, Muhannad Ahmed Obeidi, Inam Ul Ahad, Professor Dermot Brabazon, Dublin City University

Raw materials are an essential constituent for the sustainability of the economy of any industrial country. Depending upon the industry base in a country, the current and projected consumption of a particular raw material could be different. Therefore, determining the criticality level of raw materials is important. If the criticality level reaches a certain level, the material could be listed as Critical Raw Material (CRM). The European Commission via Raw Material Initiative developed the first methodology for determining the CRM list for the European Union (EU) in 2010. This methodology was reviewed and revised in 2017 and 2020. The CRM assessment methodology is primarily based on two important factors, Supply Risk (SR) and Economic Importance (EI). Supply risk covers the impact of supply restrictions and other availability factors influencing the supply chain. The EI indicates the impact on the economy if a particular raw material is not sufficiently supplied to the concerned industries. Several EU countries have adopted EU methodology and developed their CRM list. This study reviews the criticality methodology used by the EC and other European countries for the assessment of critical raw materials. Assessment methods which have been used to quantify the degree of criticality of metallic raw materials are discussed.

#### Microstructural Influence on the Fatigue Behaviour of Additively Manufactured Ti64 Alloy

Bryan Naab, University College Dublin, bryan.naab@ucdconnect.ie Dr Mert Celikin, University College Dublin & Triona Kennedy, Stryker

The advent of additive manufacturing (AM) technologies such as selective laser melting (SLM) is creating a demand for new research into how AM post-processing, such as hot isostatic pressing (HIP) and heat treatment, influences the material properties and failure mechanisms of Ti-6Al-4V. The present study examines the relationships between microstructure, processing, static mechanical properties and fatigue crack growth behaviour of Ti64 alloy produced by SLM. Furthermore, the effects of HIP and heat treatment on microstructural evolution on the fatigue crack growth behaviour were investigated via interrupted fatigue tests and Transmission electron microscopy (TEM) analysis. A direct correlation between the tensile properties with microstructure was established, however the impact toughness was determined to be mainly controlled by the porosity content rather than the microstructure.

#### Modelling the Behaviour of Irradiation-Induced Defects in Nuclear Zirconium

Jake Larkin, The University of Manchester, jake.larkin@postgrad.manchester.ac.uk Dr Chris Race, The University of Manchester & Westinghouse Electric AB

Understanding the evolution of irradiation-induced atomic defects in zirconium is an essential part of predicting the behaviour of Zr-based nuclear fuel cladding within the core of a light-water reactor. Key to this is computer modelling, where various damage scenarios can be readily simulated and isolated to develop a comprehensive picture of cladding degradation. In this study, virtual 'supercells' of 2x107 atoms are used to produce artificial 1D x-ray diffraction line profiles. These profiles are analysed for features that may help to characterise the formation and behaviour of defect loops, which consist of a ring of atomic dislocations, within the material. So far, the emergence of satellite peaks as first identified by T. Seymour et al. [1] to the high- $\theta$  side of main prismatic (100), (101), (110) Bragg peaks has been identified for interstitial <a>-type (10T0) (1st-order) loops, increasing in amplitude and reducing in proximity to the main peaks. Future work is expected to also assess the full-width half-maxima (FWHM) of these satellites and correlate them quantitatively to loop characteristics, including 2nd-order interstitial, and both 1st- and 2nd- order vacancy prismatic loops. Dislocation density  $\rho$ , representing the defect population per unit volume, will also be computed using convolutional multiple whole-profile fitting (CMWP) [2] to assess the accuracy compared to known defect concentrations.

[1] - T. Seymour, P. Frankel, L. Balogh, T. Ungar, S.P. Thompson, D. Jadernas, J. Romero, L. Hallstadius, M.R. Daymond, G. Ribarik, and M. Preuss (2017). Evolution of dislocation structure in neutron irradiated zircaloy-2 studied by synchrotron x-ray diffraction peak profile analysis, Acta Materialia, 126, p102-113. [2] - T. Ungar, G. Ribarik, M. Topping, R. Jones, X. Dan Xu, R. Hulse, A. Harte, G. Tichy, C. Race, P. Frankel, and M. Preuss (2021). Characterising dislocation loops in irradiated polycrystalline Zr alloys by x-ray line profile analysis of powder diffraction patterns with satellites. J. Appl. Crystallogr, 54, p803-821.

### Modelling the Effects of Texture on the Stress and Strain Localisation During Bending of Aluminium Alloy Sheet

Laura Gonzalez Duque, The University of Manchester, laura.gonzalez@postgrad.manchester.ac.uk Professor Joseph Robson and Professor João Quinta da Fonseca, The University of Manchester

When aluminium alloy sheets are bent, early failure can occur at grain boundaries on the surface deformed in tension. The cause of this failure is still unknown, but it has been observed that different textures lead to different propensities to failure. In this project, crystal plasticity modelling (CPM) is used to relate texture to bending failure, focusing on the effect of texture on stress and strain localisation, which is suspected to cause crack nucleation. The workflow uses the DAMASK modelling framework to model crystal plasticity, the Python package "formable" to design the load case and for parameter fitting, and MTEX for texture calculations. The inputs are textures measured with Electron Backscatter Diffraction (EBSD) and experimental tensile test curves. Uniaxial and plane strain tension load-cases, both to 15% strain, were applied to a Representative Volume Element (RVE) to simulate tension in pre-stretching and bending of three different textured samples. The stress and strain tensors at every point of the RVE were extracted and visualised using Paraview. Non-uniform stress and strain distributions were found, and the plane strain tension load-case reached higher stress and strain. However, small differences were found between three different textured samples at these low strain levels. Nonetheless, these results are the starting point to develop a model capable of predicting the effects of microstructure on failure in bending. Future work will extend the simulations to larger, more representative strains. Grain shape, texture gradients, voids and hard particles, which could also have a strong influence in the initialisation of cracks, will be considered later.

#### **Modelling the Microstructure Evolution of Titanium Alloys**

Guy Bowker, The University of Manchester, guy.bowker@postgrad.manchester.ac.uk Dr Pratheek Shanthraj & Professor Joao Quinta da Fonseca, The University of Manchester

The demand for higher quality dual-phase titanium alloy components in aerospace applications has sparked industry and academic research, focusing on the micro-mechanics taking place which affect crystallographic texture during high temperature processing. An understanding of the microstructure evolution occurring would allow for the creation of components tailor-fitted to their application. It is well understood that titanium alloys possess an anisotropic deformation response caused by HCP  $\alpha$ phase possessing strong crystallographic texture, which is undesirable. The cause for this observed texture in the  $\alpha$ -phase during hot-working is unknown. Modelling work in literature has shown that this texture cannot be easily explained by a variant-selective phase-transformation mechanism, and that the co-deformation of the two phases is much more complex than that of a soft β phase flowing around a hard  $\alpha$ -phase. It is hypothesised that dynamic phase transformation in combination with codeformation of neighbouring orientation-correlated grains contribute to this texture development. To test this, texture measurements of a dilatometer compressed sample have been compared to predictions of a replica full-field crystal plasticity model and validated against flow stress curves from literature. As expected, regions of high misorientation observed in the experimental sample were not predicted by the model. This model is now undergoing novel improvements to validate single crystal plasticity parameters of both phases against an in-situ hot compression beamline experiment

#### Molecular Dynamics (MD) Simulation of TWIP/TRIP Metals and Alloys

Mehran Bahramyan, Dublin City University, mehran.bahramyan2@mail.dcu.ie Dr James G. Carton and Professor Dermot Brabazon, Dublin City University

Twinning-induced plasticity (TWIP) and transformation-induced plasticity (TRIP) alloys are among the most promising types of metals and alloys used for various types of applications such as energy-saving and biomedical applications. These alloys generally have a high level of energy impact, thanks to the evolution of twins and dislocations during deformation as well as the phase transformation that may occur when a loading, unloading, heating or cooling process is applied. Therefore, a high level of energy is required for the fracture of these alloys. Generally, both the TWIP and TRIP mechanisms can result in uniform plastic deformation, thereby avoiding undesirable early or sudden rupture. That is why they are used for applications where collisions, explosions and other types of high-rate compression or tensile loading occurs. High entropy alloys (HEAs), stainless steels (SS), Titanium alloys, Nickel-based superalloys, Mn-steels and NiTi alloys (nitinol) are materials which exhibit TWIP and/or TRIP behaviour. It is very difficult experimentally to study the nanostructure of such alloys during deformation to extract the real-time atomic deformation mechanisms which could lead to better alloy designs for industrial applications. Thus, researchers have used reliable simulation techniques to study the twinning evolution and all types of interactions between twins and defects as well as all types of phase transformations during tensile/compression. The purpose of this study is to investigate the TWIP/TRIP mechanisms at the nanoscale using a reliable simulation approach such as molecular dynamics (MD) simulation.

#### Order-Disorder Transformation Control in AlTiVCr-Based High Entropy Alloys

Panagiotis Stavroulakis, The University of Sheffield, ppstavroulakis1@sheffield.ac.uk Professor Russell Goodall, The University of Sheffield & Tilmann Plorin, Volswaken, Wolsburg

High-entropy alloys (HEAs) push the boundaries of high-stiffness lightweight alloy design through their exceptional chemical diversity. Specifically, refractory HEA compositions have shown great promise as their specific stiffness surpasses that of even the more advanced high-modulus steels. A common occurrence in BCC refractory HEAs is their limited ductility due to the complete or partial transformation of the high-temperature BCC solid solution (A2) to the BCC B2 ordered phase at lower temperatures. A series of heat treatments have been proposed in the literature to control the formation of the ordered phase and achieve a proper balance between strength and ductility. It has also been shown that altering the chemical composition may enable further stabilisation of the A2 at the expense of B2. In this work we investigate such pathways to tackle problems evident in AlTiVCr-based systems. The associated experimental work involved manufacturing a series of alloys through Vacuum Arc Melting (VAM), subjecting them to a series of heat treatments and evaluating them in terms of their microstructural characteristics and mechanical properties.

#### **Producing Precious Metal Doped Stainless Steels by Spark Plasma Sintering**

Natasha Sweeney Fort, The University of Sheffield, nefort1@sheffield.ac.uk

Dr Richard Thackray, The University of Sheffield, Hugh Hamilton, Johnson Matthey, Gill Thornton
Liberty Powder Metals

The corrosion resistance of stainless steels can prove inadequate in oxygen-deficient acidic environments, such as within electrowinning cells. Literature shows that cathodic modification with precious metals by bulk alloying or coating can improve the corrosion resistance of stainless steels. Due to the large amounts and high costs of the precious metals used, these techniques have not

achieved commercial success. Research which explores the use of spark plasma sintering (SPS) or other powder processing techniques to produce precious metal doped stainless steels remains lacking. This project aims to incorporate precious metals into stainless steels by functional grading using SPS in an effort to reduce the volume of precious metals used to achieve cathodic modification and lower costs. The metal powders used in this project have been characterised by particle size analysis and SEM. The sintered parts have been analysed using optical microscopy to investigate porosity. Indentation testing and density measurements of the sintered samples was also carried out.

#### Pulsed Laser Ablation in Liquid for the Fabrication of Magnesium and Carbon Nanoparticle Inks Anesu Nyabadza, Dublin City University, anesu.nyabadza3@mail.dcu.ie Prof Dermot Brabazon & Dr Ronan Murphy Dublin City University, Brian Fitzpatrick, Oriel

Herein, a controllable, customisable and time-efficient fabrication method for producing C and Mg nanoparticles (NPs) of various sizes (1-2500 nm) via Pulsed Laser Ablation in Liquid (PLAL) was demonstrated. NPs provide high electrical conductivity, large surface area, high reactivity, properties which enable applications such as device size reduction for microelectronics and tailored drug delivery. NPs are conventionally synthesised via wet chemistry techniques (e.g., thermal decomposition and sol-gel method) which often require long hours of processing, hazardous chemicals, the need to purify the NPs after synthesis, highly skilled chemists, and sophisticated apparatus. PLAL involves the use of a laser to irradiate a target submerged in a liquid to produce NPs. This method is straightforward and cost-effective, requiring low-powered pulsed-lasers and can provide high production rates. Currently, PLAL research involves the investigation of laser parameters (e.g., fluence or pulse width) on the resulting colloid and these were investigated for C and Mg colloid formation to add to the existing knowledge. DI water produced smaller C NPs (10 - 82 nm) than ethanol (60 - 143 nm) and the magnesium-based solution (263 – 1389 nm). All Mg NP samples synthesised at 2 min ablation time produced a bimodal NP size distribution and bimodal distributions were only observed for 2 min ablation times. An increase in ablation time from 2 to 5 minutes changes the distribution from being bimodal (100 % of the samples) to mostly skewed (66 % of the samples) and some normally distributed (46 %). A further increase in ablation time from 5 to 25 minutes changes the distribution from being mostly skewed (66 % of the samples) to being mostly normal (56 % of the samples). It was concluded that the ablation time chiefly influences the NP size distribution.

# Spreading Area Measurements of Sn-Ag-Cu Lead Free Solder on Silver and Copper Substrates Wunmi Olukoya, The University of Sheffield, Oolukoya1@sheffield.ac.uk Professor Russell Goodall, The University of Sheffield & Edwin Raj, Johnson Matthey

The evolution of solder material has been influenced by changes in substrate materials and government initiatives to reduce lead usage. This has allowed researchers to better understand the fundamental mechanisms that govern solder joint formation, paving the way for improved material and mechanical properties in the joint. One of the most commonly used lead-free solder alternatives is the 96.5Sn-3Ag-.5Cu (SAC305) ternary metal. SAC305 has one of the lowest melting points and moderate strength characteristics on copper and nickel substrates, according to previous research. The primary difficulties with SAC305 and other lead-free solder alloys stem from the brittle intermetallic compounds that form at the solder/substrate interface. In this work, we are seeking to investigate the wetting properties of SAC305 solders on silver and copper substrates. Through in-situ observation using the Linkam TS1200, we determined that SAC305 spread more readily on the Ag

substrate than on the Cu substrate. EDX observations of the interface between the Ag/SAC305 solder showed the dissolution of the Ag substrate and the formation of Ag3Sn.

#### The Development of a Rapid CCT Predictor for Low Alloy Steels

Joshua Collins, The University of Manchester, joshua.collins@postgrad.manchester.ac.uk Dr Ed Pickering, The University of Manchester & Rolls Royce

It is well understood that alloy processing has a direct impact on steel performance. By manipulating transformation kinetics, alloy behaviour can be modified to produce unique properties unlike those predicted under equilibrium. It is this relationship that grants the ability, and the ambition, to model steel behaviour and predict the performance of processed components. A model for predicting the continuous cooling transformation (CCT) behaviour of low alloy steels has been developed using modified semi-empirical equations by Kirkaldy and Venugopalan. The model is unique in that it considers the effects of carbon partitioning on subsequent transformations, allowing it to predict characteristic CCT behaviours, like martensite suppression, that are not considered in other models. The accuracy of the model has been determined through comparisons with experimental dilatometry data. Once validated, the model can then be used to predict the microstructure and performance of steel components.

### The Evolution of Microstructure and Toughness in Multipass Welds that Contain Acicular Ferrite Enn Veikesaar, The University of Manchester, enn.veikesaar@postgrad.manchester.ac.uk

Dr John Francis, The University of Manchester & Dr Miguel Yescas, Framatome

The precise effect of chemical composition on the microstructure of welds has not been fully characterised due to the extreme amount of data and study required. Research has shown that nearly every element that is studied influences the microstructure and properties, even at trace amounts. A Bayesian neural network was used on a unique data set to produce models capable of predicting various properties of Charpy curves relative to weld composition. Models were created to predict full Charpy curves based on composition (16 elements in total and with microalloy (Ti, B, Al, N, O) isolation), predict how composition affects the upper shelf start point and how the transition point is related to the upper shelf start point. It was found that it is possible to predict unseen compositions using the created models with relatively high accuracy. We also opted to study the Ti-B-Al-N system for a set of well-characterised C-Mn HSLA steel weld samples. Optical microscopy and EBSD analysis shed light into the elusive nature of the relationships between chemical composition, microstructure and toughness.

### The Influence of Prior Deformation and Creep Asymmetry on Stress Relaxation and FE Modelling of Creep Age Forming AA2139 Plate.

Kevin Tanswell, The University of Manchester, kevin.tanswell-3@postgrad.manchester.ac.uk Thomas Jailin, Pratheek Shanthraj & Professor Phillip Prangnell, The University of Manchester, Sjoerd Van-der-Veen, Airbus Operations SAS, Toulouse, France.

Creep Age Forming (CAF) is being extended to 'fine-tune' the shape of integral airframe components, pre-formed by High Energy Hydro Forming (HEHF) to achieve cost and weight savings by reducing assembly and joining operations. In CAF dislocation creep accumulates simultaneously with precipitation and a complex interplay exists, as age-hardening progressively inhibits the creep strain build-up. A transformation strain can also occur during precipitation and the dynamic ageing conditions can influence precipitation. In addition, alloys can exhibit a 'memory' of the prior

deformation, which can affect the precipitation kinetics, precipitate distribution, and creep response. All these factors can lead to tensile-compressive anisotropy in the creep response and influence the accuracy of models used to predict the final component shape. In this work, the Creep Age Forming (CAF) response of High-Energy Hydro-Formed AA2139 sections was investigated. A combination of elevated-temperature tensile-compressive uniaxial and 4-point bending, stress-relaxation, tests and microstructural characterisation throughout the ageing sequence, has been used to deconvolute the dominant effects that control the component shape. It is shown that the deformation history can have a large effect on the creep response. In particular, strain path changes can result in significant tension-compression asymmetry in the stress relaxation. The saturation stress was found to be linearly dependent on the applied load and load reversal was found to accelerate the stress relaxation while leaving the saturation stress unaffected. A CAF constitutive model has been developed, incorporating back stresses due to strain-path changes in addition to the dislocation, solid-solution and precipitation hardening due to the microstructural evolution. The model is implemented in a finite element analysis solver and is used to predict the spring-back of geometrically complex hydro-formed components.

### The Use of Nanosecond Pulsed Laser Modification for the Increased Lifetime of a Commercially Used Pulsed Electric Field (PEF) System

Mark Swayne, Dublin City University, mark.swayne2@mail.dcu.ie Professor Dermot Brabazon, Dublin City University Laurence McDermott, Pro Stainless

The purpose of this project is to address the difficulties associated with the performance of pulsed electric field electrodes (PEF) used in processing vessel applications. The corrosion and fouling of PEF electrodes are a common problem that occurs as a result of the electrochemical reactions that take place during the process. PEF electrode corrosion results in the release of small quantities of metal from the electrodes, which mix with the fluid. Electrode corrosion in PEF is caused by the corrosion of the electrodes. This project is concerned with the development of surface modification techniques using lasers in order to improve the antifouling and anticorrosion properties of PEF electrodes. Commonly, two different methods have been employed to enhance these properties using the laser process. One is laser texturing, and the other is laser surface treatment. The laser texturing will reduce the surface roughness of the piece and increase its wettability, which has a high correlation to the antifouling properties of the metal surface. While laser surface treatment will alter the passivation layer of the stainless steel, its composition and thickness will change, leading to increased corrosion resistance. This paper presents an investigation into the effect of thin film oxide layers, which are produced by laser surface processing, on the corrosion resistance of AISI 316L stainless steel, as well as their application in a real-world application of the pulsed electric field system (PEF). A 3.5 W Nd:YAG pulsed laser, readily accessible on the market, was used to complete the project. The results of a twofull-factorial Design of Experiment (DOE) and ANOVA analysis showed that overall surface energy and hatching distance were the two most important factors influencing the corrosion resistance of colourmarked stainless-steel films. The pulsed electric field system was then used to put these laser-modified samples to use in a real-world setting. First, the impact of the PEF process parameter was examined using a central composite face-centred DOE, which changed the frequency, pulse width, and voltage parameters. Waveforms from this system are also extracted and can be used to demonstrate a considerable influence on voltage-to-current phase shift, while altering frequencies from high to low. In order to determine the difference in metal ion concentration between laser processed and unprocessed samples, the ICP-MS technique will be used to investigate the influence of these laser processed samples. This will show a direct improvement from the unprocessed to processed samples.

#### **Tool Wear in CVD Coated Carbides when Machining Ni-Based Superalloys**

Henry Boyle, The University of Sheffield, hrboyle1@sheffield.ac.uk Professor Martin Jackson, The University of Sheffield, Susanne Norgren, Sandvik Coromant AB

The wear of CVD Alumina coated Tungsten Carbide (WC) tools was investigated using a combination of static diffusion couples and machining trials, to better understand the difference in wear behaviour between wrought and powder metallurgy (PM) processed Ni-based superalloys. The alloys studied were Inconel 718 (wrought) and RR1000 (PM). Results of the static diffusion couples indicate that the variations in chemistry between these two alloys lead to the formation of entirely different species at the interface between tool and workpiece, this may explain differences in observed wear phenomena. The analysis of the machining trials remains ongoing; however, it has been observed that short tool engagement times can be used (<40s) to study the initial wear prior to coating failure. This finding demonstrates that coating wear in Ni-based superalloys can be generated using small amounts of material, which is highly advantageous for the study of these costly aerospace alloys. Novel methods of wearing tool coatings using small samples were also developed for potential use in future trials.

#### **Ultrashort Laser Sintering of Metallic Nanoparticle Inks on Heat Sensitive Substrates**

Ayesha Sharif, National University of Ireland Galway, a.sharif1@nuigalway.ie Alex Wilson, Dr Fabio Scenini, Professor Phillip Prangnell, University of Manchester

The fabrication of low cost and mechanically robust flexible electronic patterns have increasingly gained much more interest due to their growing applications in flexible displays, touch screen panels and solar cells. This requires a cost-effective sophisticated deposition of metals in a well-controlled manner with a reduced quantity of the material. Using an acoustic micro dispenser (PolyPico technologies) with a 20 picolitre droplet volume, we demonstrate room temperature printing of silver (Ag) nanoparticle (NP) ink on flexible, heat sensitive, porous substrates. Recently we have reported improvements to the crystallinity of gold, molybdenum, indium tin oxide, and amorphous silicon thin films by ultrafast laser exposure [1-4]. Compared with longer pulse durations, ultrashort pulses are characterised by their higher peak intensities, low heat affected zones, and interactions with materials on a time scale faster than that with which the laser energy is transferred to the lattice [5]. In particular, the time frame in which a higher electron temperature is established without changing the lattice temperature, we propose is important for solid state sintering of printed materials. We report the ultrashort laser-based annealing of Ag NPs inks and metallic thin films without damaging the substrate underneath. This facile, precise technique is efficient in producing highly conductive metallic patterns in a selective manner using laser fluences below the damage threshold. The reported direct low fluence ultrashort-pulse sintering is effective and promising to produce highly electrically conductive metal thin films on heat sensitive substrates for their improved applications in flexible printed electronics.

### Understanding the Effect of Strain on Microstructure Properties and Environmental Degradation of AGR Fuel Cladding

Alexander Hanson, The University of Manchester, alexander.hanson@postgrad.manchester.ac.uk

Dr Dirk Engelberg & Dr Enrique Jimenez-Melero, The University of Manchester, Ronald Clark, National

Nuclear Laboratory, Stonehouse, Gloucestershire, GL10 3UT

AGR fuel is contained within 20%Cr/25%Ni/Nb stainless steel cladding, which acts as a corrosion resistant barrier to fission product release. In non-pH moderated storage ponds, radiation-induced segregation may render the fuel cladding susceptible to intergranular corrosion, due to prior service in the reactor. This provides the potential for intergranular stress corrosion cracking, at locations on the fuel pin previously strained during fabrication or service. Limited research is available on stresscorrosion cracking behaviour of AGR fuel cladding; however, a thorough understanding of potential degradation mechanisms is required. This study aims to address this by investigating how changes in strain and cold work of 20%Cr/25%Ni/Nb can impact microstructure, localised corrosion behaviour and consequently stress corrosion behaviour. Current work focuses on development of the use of digital image correlation with a micro-tensile stage, combined with electrochemical control; for realtime imaging of cladding microstructures exposed to storage relevant environments. This allows observation of local strain developments in the microstructure and potential crack formation under applied stress, whilst electrochemical measurements are taken to understand corrosion performance. The goal is to determine where cracks initiate, and if they can be inhibited, to understand if changes in local microstructure strains play a key role in spent fuel failure. Development and characterisation of calcium phosphates coating layers on magnesium substrates for control the degradation rate and enhance the bone repair for potential orthopaedic implantation applications

#### Weldability of Novel High Entropy Alloys for Selective Laser Melting

Lucy Farquhar, The University of Sheffield, laufarquhar1@sheffield.ac.uk Professor Russell Goodall, The University of Sheffield & Lukas Jiranek, Boeing

In this work an assessment of weldability is proposed in order to ascertain the suitability of novel high entropy alloys for AM, using small arc-melted samples, prior to any powder manufacture. This aims to result in a method by which to assess if an alloy will be able to be manufactured by AM without cracking, before the costly step of producing powder and completing the AM process itself. Weld tracks were completed on 3 CoCrFeNi based HEAs which had previously been manufactured through AM and showed varying weldability and crack susceptibility. The same weld tracks and analysis was completed on some novel high entropy alloys, designed by theoretical modelling. Along with theoretical equations and comparison with known alloys, the suitability of the novel HEAs for AM was predicted and the novel HEA compositions which show good weldability are then further characterised.

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