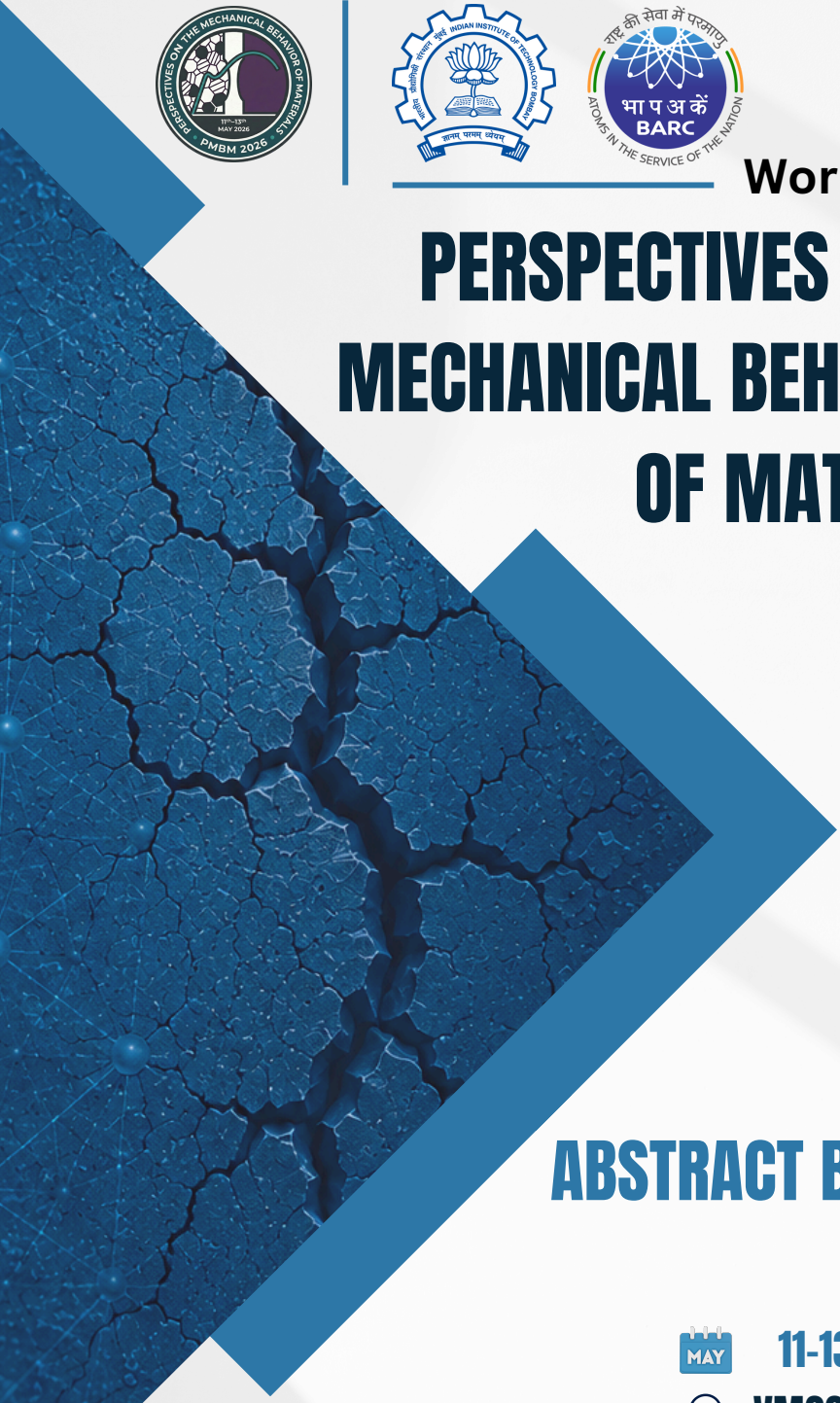
Workshop on

PERSPECTIVES ON THE MECHANICAL BEHAVIOUR OF MATERIALS



ABSTRACT BOOKLET

11-13 MAY, 2026

VMCC, IIT BOMBAY

WORKSHOP SCHEDULE

Day 1: 11 May, 2026
Venue: Hall No. 22, 2nd Floor, VMCC Building, IIT Bombay

Time	Session
08:30 – 09:00	Registration and Breakfast
09:00 – 09:10	Introduction to the workshop
09:10 – 09:50	**Advances in mechanical characterization** **Prof. Subramanya Sarma, IIT Madras** Effect of strain rate on the retained austenite stability in a Medium-Mn steel
09:50 – 10:30	**Prof. Nilesh Gurao, IIT Kanpur** Deformation twinning in uniaxial and sequential compression of Mg-0.5 wt.% Ce alloy
10:30 – 11:10	**Prof. Sudarshan Phani, University of Hyderabad** High throughput nanoindentation testing: the new paradigm in small-scale mechanical testing
11:10 – 11:40	Tea / Coffee Break
11:40 – 12:20	**Dr. V. Karthik, IGCAR, Kalpakkam** Recent advances in small punch testing for evaluating tensile, fatigue and fracture properties
12:20 – 13:00	**Prof. Eswara Prasad, IIT Indore** Investigating the mechanical behavior of magnesium using in-situ experiments: Insights into deformation twinning
13:00 – 14:20	Lunch
14:20 – 15:00	**Microstructure engineering through deformation methods - I** **Prof. Suresh Neelakantan, IIT Delhi** Engineering microstructures via martensitic transformation for enhanced mechanical properties in metastable β titanium alloys
15:00 – 15:40	**Prof. Devinder Yadav, IIT Patna** Furnace-free electric-field-induced high strain rate superplasticity in 3YSZ
15:40 – 16:20	**Prof. Sanjib Acharya, Jadavpur University** High-temperature fatigue crack growth behavior of structural materials: mechanistic understanding and experimental analysis
16:20 – 18:30	Tea / Coffee + Posters

Day 2: 12 May, 2026
Venue: Hall No. 22, 2nd Floor, VMCC Building, IIT Bombay

Time	Session
09:00 – 09:40	**Computation of deformation mechanisms in materials** **Prof. Anand Kanjarla, IIT Madras** Microstructure informed crystal plasticity modelling of low cycle fatigue behavior of IN718
09:40 – 10:20	**Prof. Anirban Patra, IIT Bombay** Scale Bridging Strategies for Computationally Efficient Prediction of Anisotropic Deformation at the Mesoscale and Macroscale
10:20 – 10:50	Tea / Coffee Break
10:50 – 11:30	**Prof. Suchandrima Das, IISc Bangalore** A Multiscale Framework for Deformation in Defect-Rich Materials: Bridging CPFE and Atomistic Simulations_
11:30 – 12:10	**Abhik Chaudhury, IISc Bangalore** Towards intrinsically coupled microstructure informed damage models for the prediction of creep life in Ni-based superalloys
12:10 – 12:50	**Prof. Rajeshwar Eleti, IIT Roorkee** Electronic-structure governed strengthening in face-centered cubic high-entropy alloys: A unified framework for solid-solution and grain size strengthening mechanisms
12:50 – 13:05	**Industry talk – Maximator India Pvt. Ltd.**
13:05 – 14:20	Lunch
14:20 – 15:00	**Deformation, Processing and Degradation of Nuclear Structural Materials** **Dr. R. N. Singh, BARC Mumbai** Mechanical properties evaluation and its application for safety assessment of internally pressurized components.
15:00 – 15:40	**Dr. M. Vasudevan, IGCAR Kalpakkam** Strategies for Enhancing the Creep Strength of Ferritic-Martensitic Steels and their Weld Joints
15:40 – 16:20	**Prof. Satyam Suwas, IISc Bangalore** Dwell Fatigue in Titanium alloys

Day 3: 13 May, 2026
Venue: Hall No. 22, 2nd Floor, VMCC Building, IIT Bombay

16:20 – 16:50	Tea / Coffee Break
16:50 – 17:30	**Prof. Ankur Chauhan, IISc Bangalore** Exploring the Irradiation Response of Multi-Principal Element Alloys: Insights from Proton-Induced Defect Dynamics and Recovery
17:30 – 18:10	**Dr. Rajeev Kapoor, BARC Mumbai** Physics-based constitutive framework for α-Zr alloys deformed at low to warm temperatures and across quasi-static to dynamic strain rates
18:30 – 21:00	Dinner + Poster Awards

Day 3: 13 May, 2026
Venue: Hall No. 22, 2nd Floor, VMCC Building, IIT Bombay

Time	Session
09:00 – 09:40	**Microstructure engineering through deformation methods – II** **Prof. Debalay Chakrabarti, IIT Kharagpur** Thermomechanical simulation of grain structure evolution in steels
09:40 – 10:20	**Prof. K. V. Vamsi, IIT Indore** Modelling Deformation Pathways in Ordered Alloys via Planar Fault Energetics
10:20 – 11:00	**Prof. Shanta Chakrabarty, KIIT Bhubaneswar** Tailoring microstructure and texture evolution through strain path in low-Ni austenitic stainless steel
11:00 – 11:30	Tea / Coffee Break
11:30 – 12:10	**Materials under extreme conditions and environments** **Dr. Vani Shankar, IGCAR Kalpakkam** Analysis of fatigue hysteresis loops to understand the evolving microstructures of high temperature materials under various cyclic loading waveforms
12:10 – 12:50	**Prof. R. S. Kottada, IIT Madras** Creep of additively manufactured Ni-base superalloys
12:50 – 14:20	Lunch
14:20 – 15:00	**Prof. Dhiraj Mahajan, IIT Ropar** Perspectives on Hydrogen-Assisted Fatigue Crack Initiation in Metals using Small-Scale Experiments and Crystal Plasticity Simulations
15:00 – 15:40	**Prof. Niraj Chawake, IIT Kanpur** Effect of Ti Addition on Screw-Dislocation Mediated Plasticity in W-Containing Refractory High-Entropy Alloys
15:40 – 16:40	High Tea + Discussion (What did we learn and the way forward)

ABSTRACTS

SCALE BRIDGING STRATEGIES FOR COMPUTATIONALLY EFFICIENT PREDICTION OF ANISOTROPIC DEFORMATION AT THE MESOSCALE AND MACROSCALE

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ABSTRACT

Mesoscale crystal plasticity models are the state-of-the-art for predicting the anisotropic and heterogeneous deformation of metallic systems as a function of the underlying microstructure. Specifically, full field crystal plasticity models can predict the effects of crystallographic texture and grain morphology, which may develop during thermo-mechanical processing, on the anisotropic deformation behavior. However, these models are generally associated with significant computational costs, which limit their applications for simulating the deformation of components. In this talk, we discuss two ongoing efforts in our group on developing scale bridging strategies for computationally efficient prediction of anisotropic deformation.

Using predictions from our full field crystal plasticity model as the reference, we use identical constitutive equations and parameters for dislocation density-based strengthening and evolution in a mean field elasto-visco-plastic crystal plasticity model for predicting the anisotropic deformation of dual phase steels. A new linearization scheme is proposed in the mean field crystal plasticity model to account for the intergranular interactions. Intragranular stress distributions are also introduced in the mean field crystal plasticity model to represent the heterogenous deformation generally observed within grains in the full field model. The computationally efficient mean field crystal plasticity model is used for predicting the anisotropic yield/flow surfaces of two different dual phase steel grades.

In another study, we attempt to derive constitutive model parameters in a macroplasticity model from our full field crystal plasticity simulations. Identical constitutive equations are used in both models, while necessary scaling of the model parameters is performed at the macroplasticity level to predict the anisotropic deformation of a ferritic steel and an Al alloy subject to biaxial loading.

We discuss challenges and limitations of these scale bridging strategies, as well as their potential for performing component simulations.

Keywords: crystal plasticity, anisotropic deformation, macroplasticity, dislocation densitiy

TOWARDS INTRINSICALLY COUPLED MICROSTRUCTURE INFORMED DAMAGE MODELS FOR THE PREDICTION OF CREEP LIFE IN NI-BASED SUPERALLOYS

Abhik Choudhury, Shubham Mridha, Pushkar Pandit, Achyut Kumar, Saswata Bhattacharyya and, The MicroSim Team

ABSTRACT

Creep is the principal damage mechanism leading to the failure of turbine blades in the high pressure turbine (HPT) stage of an aeroengine as well as pressure tubes in steam driven power plants. Design for newer alloys is limited by the accuracy in the prediction of creep life. While damage models exist, the coupling of these models with the evolution of the microstructure metrics during operation is limited, and needs to be more robust for the better prediction of creep-life. In this talk, I will elaborate on the physical pheonomena determining creep life and the integration of evolution metrics derived from phase-field simulations with damage models. I will demonstrate the usage of MicroSim (https://github.com/ICME-India/MicroSim) for the simulation of microstructure evolution at elevated temperatures in the presence of stress for real Ni-based alloys by coupling with information from thermodynamic databases. The microstructure metrics related to precipitate sizes and channel spacings are fed into damage models such as the Dyson and Mclean [1] using which creep-life predictions are made. The predictions reveal the influence of stresses on the creep life.

While these results are encouraging, I will highlight the knowledge gaps that limit the broader applicability of these results for real world applications. One of them is the role of activated dislocation driven plasticity in determining creep life and thermodynamically consistent formulations for incorporating plasticity-mediated microstructure evolution in phase-field simulations. Along with this, the lack of accurate diffusivity matrices, contributes to the uncertainity in the predictions from these models. I will elaborate on some of our efforts in these directions.

[1] M. McLean, B. F. Dyson, Journal of Engineering Materials and Technology. 122, 273–278 (2000)

EFFECT OF TI ADDITION ON SCREW-DISLOCATION MEDIATED PLASTICITY IN W-CONTAINING REFRACTORY HIGH-ENTROPY ALLOYS

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ABSTRACT

Refractory high-entropy alloys (RHEAs) based on group-V and group-VI transition metals are promising candidates for extreme-environment applications, including plasma-facing components in fusion reactors, owing to their high melting temperatures and radiation tolerance. However, the practical use of tungsten-containing RHEAs with a body-centered cubic (BCC) crystal structure is severely limited by their intrinsic brittleness at room and relatively low temperatures. Consequently, improving the ductility of BCC RHEAs remains a critical challenge. Plastic deformation in BCC metals and alloys is primarily governed by the mobility of ½<111> screw dislocations, which therefore play a decisive role in determining their plasticity.

In this work, we investigate the effect of a minor Ti addition (5 at.%) on the intrinsic ductility of the W-containing RHEA, W0.36Ta0.36Nb0.28, using density functional theory (DFT) in conjunction with experimental techniques. DFT calculations show that Ti addition promotes a non-compact dislocation core configuration and reduces the Peierls barrier, thereby facilitating screw-dislocation motion. Consistent with these predictions, experimental results reveal enhanced plastic strain and increased screw-dislocation mobility. Dislocation structures were further characterized using controlled electron channeling contrast imaging (cECCI). Long, straight screw dislocations were observed in W0.36Ta0.36Nb0.28, whereas cusped dislocations were identified in (W0.36Ta0.36Nb0.28)Ti0.05. The Ti addition promotes the formation of superjogs, which act as temporary pinning points and contribute to simultaneous improvement in strength and ductility. This behavior closely resembles the ductilizing effect reported in W–Re alloys. Slip-trace analysis further reveals that deformation in the base RHEA is dominated by {110} slip, while Ti addition activates {112} slip systems and promotes frequent cross-slip. These findings establish the operative deformation mechanisms responsible for the improved ductility in Ti-modified W-containing RHEAs.

ANALYSIS OF FATIGUE HYSTERESIS LOOPS TO UNDERSTAND THE EVOLVING MICROSTRUCTURES OF HIGH TEMPERATURE MATERIALS UNDER VARIOUS CYCLIC LOADING WAVEFORMS

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ABSTRACT

Fatigue behaviour of materials is an important consideration for evaluating safety of operating structures as almost 90% of the service-related failures occur by fatigue loadings. Combined fatigue and creep loading is more deleterious than either of them acting alone and in real scenario the loading waveforms can be even more complex. For the component's safe service performance and reliability at high temperature and extreme service environment, a thorough understanding of the degradation mechanisms and their quantitative analysis throughout its life is of utmost importance. Service condition often involves load temperature environment (corrosive/irradiation) combinations and hence to mimic the service conditions as close as possible, mechanical testing under combined loadings and environment are necessary.

Materials performance is highly microstructure sensitive and waveform dependent. Taking example of the occurrence of dynamic strain ageing in different high temperature structural materials, this presentation shall bring out the possibility of use of hysteresis loops to visualize the underlying microstructural evolution occurring in a range of materials under various cyclic loading waveforms. Hysteresis loop analysis obtained during fatigue experiments contain a lot of information but are often ignored due to complexity in data analysis.

Bulk materials of Grade 91, RAFM steel, 321 SS, soft iron and Alloy 617 M and thin wafers of copper and Aluminium that are subjected to various types of fatigue loading waveforms such as isothermal fatigue, creep-fatigue interaction, ratcheting and thermo-mechanical fatigue, shall be discussed. These examples shall illustrate the possibility and advancements in fatigue data processing for correlating the evolution of microstructural constituents affecting the macro deformation. The presentation would leave on the note that fatigue experiments can be used as an early-stage screening towards material selection, development and processing.

TAILORING MICROSTRUCTURE AND TEXTURE EVOLUTION THROUGH STRAIN PATH IN LOW-NI AUSTENITIC STAINLESS STEEL

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ABSTRACT

Low-Ni metastable austenitic stainless steels show an outstanding combination of strength and ductility due to the combined effect of slip and strain-induced phase transformation of γ-austenite (FCC) to α-martensite (BCC). Since both mechanisms are highly sensitive to loading conditions, understanding the effect of strain path on deformation behavior is essential for optimizing the microstructural stability and sheet metal formability. In the current study, the effect of strain path on microstructural evolution, martensitic transformation, and texture development was investigated using 0.7 mm thick low-Ni austenitic stainless-steel sheets subjected to Limiting Dome Height (LDH) testing. The microstructural analysis shows that local lattice distortion caused by slip activity was highest under Biaxial stretching (BS), followed by Plane Strain (PS) and Uniaxial (US) deformation conditions, whereas the volume fraction of α-martensite followed the opposite trend of US > PS > BS. It was also observed that the suppressed martensitic transformation under BS was due to a different texture formed during deformation. Texture analysis showed that BS deformation strongly promoted fiber texture evolution through the strengthening of Brass {110}<112> and Goss {110}<001> components, resulting in higher Orientation Distribution Function (ODF) intensity and texture index values than PS and US conditions. The correlation among strain path, active deformation mechanisms, phase transformation, and texture evolution was further used to predict the material's strain hardening behaviour. Despite these advances, accurate prediction of strain-path–dependent microstructural evolution and martensitic transformation under complex loading conditions remains a significant challenge. The combined interaction of slip, twinning, and phase transformation mechanisms is not yet fully understood. Real-time experimental characterization during deformation is still limited, especially under industrial forming conditions. The development of reliable multiscale models integrating the microstructures, crystallographic texture, phase stability, and mechanical response remains a critical area that needs further attention.

Keywords: Low-Ni austenitic stainless steels, LDH, strain path, phase transformation, texture

STRATEGIES FOR ENHANCING THE CREEP STRENGTH OF FERRITIC-MARTENSITIC STEELS AND THEIR WELD JOINTS

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ABSTRACT

Ferritic martensitic steels (9–12 wt.% Cr) are extensively used in the thermal and nuclear power plants. F-M steels have been widely used for steam generator applications because of its low thermal expansion, high thermal conductivity, resistance to stress-corrosion cracking, good weldability and adequate mechanical properties at high temperatures. Further, inherent resistance to void swelling under fast neutron irradiation environment, make it a strong candidate material for in-core applications as clad and wrapper in fast reactors. It is also chosen for application as sodium carrying pipes and intermediate heat exchangers and is also a candidate material for pressure vessel application in Lead cooled Fast Reactor (LFR). Reduced activation F-M steel (RAFM) and their variants are candidate materials for application in fusion reactor.

Grade 91 steel is a F-M steel and its application is limited to 873 K. Grade 91 steel weld joint is prone to type IV cracking and undergo premature failure during high temperature service. Worldwide, many strategies have been adopted to enhance the creep strength of the above steel and to mitigate type IV cracking in its weld joint. Modifications to composition, heat treatment, thermo-mechanical treatment (TMT) and dispersion strengthening in grade 91 steel have been carried out by us to enhance the creep strength and significant enhancement in creep strength have been achieved. In addition to modifications in composition and heat treatment, right choice of welding process have been found to enhance the resistance to type IV cracking in F-M steels. Eliminating fine grained HAZ (FGHAZ) in F-M steel weld joints would mitigate type IV cracking and is still a big challenge. Enhancing the creep strength of F-M steels however would reduce the impact toughness and it is always a challenge to achieve a trade-off between creep strength and impact toughness for applications in thermal and nuclear power plants.

Keywords: F-M Steels, TMT, Creep, weld joint, Type IV cracking

DEFORMATION TWINNING IN UNIAXIAL AND SEQUENTIAL COMPRESSION OF MG-0.5 WT.% CE ALLOY

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ABSTRACT

Deformation twinning is the most important plastic deformation mechanism after dislocation slip in crystalline materials, wherein atomic shear creates a mirror-image orientation of the crystal within the grain. It is prominent in fcc metals and alloys with low stacking fault energy and all hcp metals and alloys, and is dominant in most materials deformed at high strain rates and low temperatures. Twinning, unlike slip, is directional and causes sudden reorientation of significant volume, contributing to significant texture evolution at low global strain. The operation of deformation twinning contributes to dynamic Hall-Petch strengthening, leading to sustained strain hardening and higher ductility, but also acts as a damage nucleation site.

The present study investigates the critical role of deformation twinning in Mg-0.5 wt.% Ce alloy during uniaxial and sequential compression at room temperature using detailed microstructural and textural characterization along with mean-field and full-field crystal plasticity simulations. The cuboid sample subjected to uniaxial compression to a strain of ~0.09 shows the evolution of basal texture. In contrast, the sample subjected to sequential multiaxial compression along the three orthogonal directions to the same von Mises strain shows a weakening of the basal texture. The stress-strain curve under uniaxial loading is sigmoidal due to pronounced {10-12} extension twinning, while a stress drop is observed during a strain-path change in sequential compression due to texture softening. The sample subjected to sequential compression exhibited a lower strain-hardening rate. The uniaxial compression sample shows thick parallel twins in grains, while thin intersecting twins and twin chains were observed in sequential compression. Crystal plasticity simulations can capture the evolution of microstructure, texture and stress-strain response for both the deformation modes. The higher variations in local stresses and local Schmid factor in the sample subjected to sequential compression explain the distinct evolution of twin characteristics and weakening of basal texture compared to uniaxial deformation.

Developing a fundamental understanding of the microstructural origins of twin nucleation, propagation, and thickening by experimental techniques and crystal plasticity models remains an open challenge for the materials mechanics community.

Keywords: deformation twinning, microstructure, crystal plasticity, magnesium alloy

ENGINEERING MICROSTRUCTURES VIA MARTENSITIC TRANSFORMATION FOR ENHANCED MECHANICAL PROPERTIES IN METASTABLE β TITANIUM ALLOYS

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ABSTRACT

Stress-induced martensite (SIM) transformations in retained metastable phase are known deformation mechanisms that provide additional plasticity in several alloy systems. Metastable β titanium alloys show significant potential for microstructure modification through martensitic transformation. Typically, β(austenite)→α"(orthorhombic) and β →α' (hcp) martensitic transformations are induced in them either by quenching or application of load. The two transformations differ from each other in terms of atomic shuffle displacement, wherein former requires less displacement than the latter. Therefore, β →α" transformation can be considered as a crystallographically incomplete β →α' transformation. Further, the influence of different alloying elements in metastable β-Ti alloys also plays an important role in driving the α"→α' martensitic transformation. In addition, the microstructural state, in particular the β phase stability, in the alloy and β grain orientations also play an important role on the martensite transformation during deformation and eventual property enhancement in metastable β-Ti alloys.

The present talk will aim to demonstrate the SIM transformation in metastable β Ti-10V-2Fe-3Al (Ti-1023) alloy, resulting in achieving ~ 43% cold reduction. The evidence of phase transformation from β→α"→α' is also observed in Ti-1023 during continuous deformation. XRD analysis confirms the transformation of α″ to α′. It has been observed that the driving force for $\alpha'' \rightarrow \alpha'$ martensitic transformation is the combined effect of lattice strain induced by cold rolling and the different alloying elements. A correlation of the lattice strain and alloying elements on the transformation of $\beta \rightarrow \alpha'' \rightarrow \alpha'$ in Ti-1023 has been established. Significant fraction of stress-induced martensites provide preferential nucleation sites for new strain-free grains upon recrystallization annealing. The thermomechanical treatment resulted in grain refinement by ~ 93% in Ti-1023 alloys. Further, the effect of grain size on the SIM transformation ability based on micro hardness variations has been deduced. In addition, the role of β phase stability on the SIM transformation has been elucidated using Electron Probe Micro Analyzer (EPMA) in the Ti-1023 microstructure. EPMA confirms the role of alloying element (such as Fe, Mo, V, Cr and Al) diffusivities on the stability of the β phase as a function of recrystallization time. Furthermore, nanoindentation has been used to elucidate the relationship of grain orientation on the SIM transformation behaviour during deformation and their eventual influence on the mechanical properties of Ti-1023. Austenite grains with specific crystallographic orientations of [001], [101] and [111] have been chosen. Nanoindentation was performed with two different diamond indenters viz. Berkovich and Cono-spherical. Nanoindentation reveals dominant stress-induced martensitic (of α" type) transformation in the grains with [111] crystallographic orientation, which contrasts with [001] orientations showing only the presence of slip at the surface. The observations confirm that [111] is the most favored grain orientation, followed by [101] for enhanced SIM, while the [001] orientation is the least favoured. Overall, the study elucidates that SIM transformation during plastic deformation results in strength-ductility enhancement via transformation-induced plasticity in metastable β-Ti alloys. The main challenge still lies in extending the understanding to control such transformation behaviour and respective property enhancements, and as well the type of martensite formation, in other metastable β-Ti systems.

The speaker shall also involve the shape memory alloys to demonstrate the role of martensite transformation in mechanical property enhancement, if time permits.

Keywords: Martensitic transformation; metastable β Titanium alloys; Stress-induced transformation; Shape memory alloys; Strength-ductility.

MODELLING DEFORMATION PATHWAYS IN ORDERED ALLOYS VIA PLANAR FAULT ENERGETICS

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ABSTRACT

Planar faults such as antiphase boundaries (APBs) and superlattice stacking faults (SSFs), play a central role in controlling the mechanical response of ordered intermetallic alloys, particularly their strength and creep resistance. Accurate determination of these defect energies is therefore vital for the design of advanced structural materials. Given their central role, experimental measurement of planar fault energies remains challenging due to the nature of available techniques and the time-consuming efforts. As a result, reliable data is limited to a set of compositions and fault types. Although first-principles approaches based on density functional theory provide a rigorous alternative, the use of large supercells to explicitly model faulted configurations makes these calculations computationally expensive, particularly for multicomponent systems and at finite temperatures. This limits their applicability for the systematic exploration of composition space in new alloys. To address this gap, high- throughput approaches such as the Diffuse Multi-Layer Fault (DMLF) model have been developed to estimate planar fault energies. The model provides rapid estimates for L12 alloys and has been extended to D022 structures. Recently, the idea of discovering proximate structures that replicate the local environment of APBs in B2-ordered compounds enabled efficient, accurate predictions. Applications to refractory high-entropy alloys (RHEAs) demonstrate that the DMLF methodology serves as a computationally tractable alternative to first-principles supercell approaches. This capability enables rapid exploration of alloy compositions with desired planar fault energies, as well as understanding plastic deformation driven by stacking faults and solute segregation. The broader implication of this work is the creation of a predictive framework that integrates defect energetics into computational alloy design for next-generation high-temperature structural materials. Despite this progress, key challenges remain, particularly in bridging atomistic energetics with mesoscale evolution and experimental observations to achieve fully predictive models. This work aims to contribute toward such a unified, mechanistically informed framework for alloy design.

Keywords: Planar fault energy, DMLF model, superalloys, high-entropy alloys, alloy design

EFFECT OF STRAIN RATE ON THE RETAINED AUSTENITE STABILITY IN A MEDIUM-MN STEEL

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ABSTRACT

Medium Mn steels are one of the most promising candidates among the third-generation AHSS for automotive applications due to the enhanced strength and ductility exhibited by them. The superior mechanical properties can be attributed to their extended strain-hardening behavior which is dependent on the stability of the retained austenite present in the microstructure. The current work involves the study of the effect of a high strain rate on a medium Mn steel composition designed and developed using the CALPHAD approach to optimize critical parameters such as austenite stability and stacking fault energy [1]. The objective of this study is to understand the effect of different strain rates (10^{-3}, 1, and 10^{3} s^{-1}) on the stress-strain response and the austenite to strain-induced α′-martensite transformation under uniaxial compression. The results show an enhanced stability of the retained austenite and consequently a lower strain hardening behavior with an increase in the strain rate. This stability observed in the retained austenite can be attributed to the adiabatic heating which becomes predominant at higher strain rates and the retardation in the strain-induced transformation of the retained austenite as a function of strain rate [2]. The study aims to deconvolute and understand both possible reasons and highlight their contributions to the overall stability of the retained austenite. The challenges are the understanding stability of the retained austenite under different stress states and loading rates.

Keywords: Medium Mn steels, Retained austenite, Strain induced transformation

References

[1] A.K. Patra, C.N. Athreya, S. Mandal, K.C. Hari Kumar, V. Subramanya Sarma, High strength-high ductility medium Mn steel obtained through CALPHAD based alloy design and thermomechanical processing, Mater. Sci. Eng. A. 810 (2021) 140756.

[2] A.K. Patra, R. Kapoor, S. Mandal, K.C. Hari Kumar, V. Subramanya Sarma, High strength-high, Influence of strain rate on the work hardening, strain induced martensite formation, strain partitioning, and variant selection in a medium-Mn steel, Mater. Sci. Eng. A 902, (2024), 146593,

PERSPECTIVES ON HYDROGEN-ASSISTED FATIGUE CRACK INITIATION IN METALS USING SMALL-SCALE EXPERIMENTS AND CRYSTAL PLASTICITY SIMULATIONS

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ABSTRACT

As the global shift to hydrogen as an alternative energy carrier intensifies, hydrogen storage and transportation face critical challenges due to hydrogen embrittlement (HE). HE causes loss of ductility, strength, fracture toughness, and fatigue life in metals by drastically accelerating crack initiation, which is often the dominant phase of component life. While crack propagation is extensively studied, hydrogen-assisted crack initiation is underexplored. Multiple HE mechanisms operate simultaneously in metals, modulated by crystal structure and microstructure.

This talk will present the micromechanics of fatigue crack initiation (FCI) in metals based on in-situ small-scale experiments. The experiments involve extensive testing of model metal, nickel, during strain-controlled low-cycle fatigue (LCF) under SEM. The hydrogen-charged samples show elevated intergranular FCI via HELP-mediated HEDE revealed using the microstructural stress maps (hydrostatic/von Mises stress, triaxiality) extracted by employing novel coupling of HR-DIC and EBSD analysis at grain boundaries. A crystal-plasticity FEM based displacement-diffusion coupled framework further corroborates the finding using simulations.

These findings provide predictive models and design strategies for HE-resistant metals.

Keywords: Hydrogen Embrittlement, Stress Maps, HEDE, HELP.

MICROSTRUCTURE INFORMED CRYSTAL PLASTICITY MODELLING OF LOW CYCLE FATIGUE BEHAVIOR OF IN718

Anand K Kanjarla
IIT Madras

ABSTRACT

Mechanical response of materials measured at the macroscopic scale are manifestations of physical phenomena occurring at lower length scales, among which the most important is the mesoscale. Constitutive models developed to predict the mechanical behaviour of metallic materials should account for the multiscale nature of the problem. The most common way to do so is through what is known as crystal plasticity. Here, we present an overview of crystal plasticity and its application to modelling of low cycle fatigue behavior of Inconel 718, a high strength nickel based alloy used in critical components subjected to cyclic loading such as turbine blades and disks. Upon cycling loading, IN718 exhibits cyclic softening i.e. the stress amplitude decreases with accumulated plastic strain. Experiments show that the cyclic softening is due to the shearing of the precipitates in the material. However, existing models rarely account for precipitate shearing explicitly. We present a dislocation density-based crystal plasticity model to account for the precipitate induced cyclic softening in IN718. The model treats the interaction between precipitates and dislocations using a probabilistic approach. It is also capable of capturing the reduction in the effective size of the precipitates due to reversible dislocations shearing through them. The developed model, used to simulate low cycle fatigue, predicts the macroscopic behavior satisfactorily by capturing the initial hardening and subsequent softening during cyclic loading for several strain amplitudes. Finally, we will discuss some outstanding issues and current trends in modelling fatigue in polycrystalline materials.

Keywords: IN718, low cycle fatigue, stress softening, precipitate shearing, crystal plasticity

FURNACE-FREE ELECTRIC-FIELD-INDUCED HIGH STRAIN RATE SUPERPLASTICITY IN 3YSZ

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ABSTRACT

Flash sintering is an electric field-assisted sintering technique in which a sample densifies within a few seconds at relatively low furnace temperatures. During flash sintering, a surge in power dissipation is accompanied by a non-linear increase in the electrical conductivity of the specimen. Not only porous samples, but also dense polycrystals and single crystals exhibit the flash phenomenon, although they do not undergo densification.

This study demonstrates superplastic deformation in 3 mol% yttria-stabilized zirconia (3YSZ) induced by flash phenomena under ambient conditions, i.e., without the use of a furnace. An electric field of 100 V/cm was applied across the dog-bone shaped sample, and the flash state was triggered using a butane torch. Superplastic elongation was achieved in a current density window of 200-225 mA/mm2 under a constant applied load. Tensile creep experiments performed at room temperature revealed significant superplastic elongation, reaching ~110% at a current density of 225 mA/mm2 under a low flow stress of ~2.6 MPa. The deformation behaviour is characterized by a two-stage creep response with a dominant steady-state regime. Microstructural analysis using SEM and EBSD confirmed grain boundary sliding (GBS) to be the primary deformation mechanism at both current densities, while the accommodation mechanism transitions from dislocation activity localized in the grain boundary mantle region at lower current density to enhanced intragranular dislocation activity at higher current density. The stress exponent ($n \approx 2.1–2.3$) further supported GBS-controlled deformation. Significant dynamic grain growth and the evolution of microcavities and wedge cracks were observed, indicating GBS. The results highlight the role of electric-field-induced defect generation in enhancing diffusion kinetics and reducing flow stress. Importantly, the ability to induce and sustain flash in dense ceramics using a simple external heat source enables rapid, high strain rate superplastic deformation and facilitates shape modification of ceramic components.

Keywords: Flash phenomena, Superplasticity, Zirconia, Grain boundary sliding

HIGH THROUGHPUT NANOINDENTATION TESTING: THE NEW PARADIGM IN SMALL-SCALE MECHANICAL TESTING

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ABSTRACT

High speed nanoindentation mapping has emerged as a powerful tool to measure the local mechanical properties with high throughput. Advancements in instrumentation, test methodology and analysis techniques have enabled fast measurements without compromising the reliability of the data. These advancements have now resulted in generating large indentation data sets on small volumes of materials, which can be analyzed with advanced statistical tools to quantitatively determine the properties of individual phases in a multi-phase alloy.

In this talk, an overview of high speed nanoindentation testing will be presented with specific focus on the various factors that determine the precision and accuracy of the measured data. Additionally, results of high speed nanoindentation mapping coupled with microstructural analysis using SEM/EBSD will be presented to demonstrate the power of correlative characterization at the micrometer length scale. Finally, 4D High-Speed Nanoindentation Mapping methodology that enables high-throughput spatially resolved mechanical mapping far beyond conventional indentation mapping methods will be presented to demonstrate how nanoscale heterogeneities, interfaces, and gradients control macroscopic mechanical response.

Keywords: Nanoindentation, high speed mapping, data deconvolution, correlative characterization

THERMOMECHANICAL SIMULATION OF GRAIN STRUCTURE EVOLUTION IN STEELS

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ABSTRACT

The grain structure plays a critical role in determining the mechanical properties of metallic alloys. The formation of coarse or mixed (coarse + fine) grain structures often degrades properties such as impact toughness. Therefore, achieving a fine and uniform grain structure is essential for optimal mechanical performance.

This lecture will address the influence of thermomechanical processing on grain structure evolution in steels, along with key challenges associated with industrial processing and the resulting microstructural features.

A major emphasis will be placed on thermomechanical simulation. It is well established that heavy finishing deformation at relatively low temperatures promotes the formation of fine and ultrafine ferrite grain structures, thereby enhancing strength through grain boundary strengthening. Systematic simulations were conducted using the Gleeble®3500 system by varying deformation temperature, strain per pass, and inter-pass time. Both single-pass and multi-pass deformation schedules were explored to replicate industrial rolling conditions. The hot flow curves will be analyzed to elucidate microstructural restoration mechanisms. In addition, a mathematical framework for predicting the full grain size distribution during thermomechanical processing will be presented.

Finally, novel thermomechanical schedules were also designed to generate mixed (bimodal) grain structures, and the influence of these grain structure variations on mechanical properties will be discussed.

Keywords: Thermomechanical Processing, Deformation Simulation, Grain Size Distribution, Hot-Flow Curves, Ultrafine Grain, Mixed Grain Structure.

RECENT ADVANCES IN SMALL PUNCH TESTING FOR EVALUATING TENSILE, FATIGUE AND FRACTURE PROPERTIES

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ABSTRACT

The Small Punch Test (SPT) is a miniature specimen technique with strong potential for evaluating mechanical properties in situations where material availability is limited and conventional-sized specimens cannot be obtained. The method involves deforming a thin specimen, typically about 0.5 mm in thickness, clamped between a set of dies, using a hemispherical punch, while continuously recording the load–deflection response for subsequent analysis of mechanical behavior. The complex stress state and deformation behavior in the small punch test make the interpretation of results and their correlation with conventional mechanical properties more challenging.

The presentation will highlight recent advances in small punch test and analysis methodologies, towards reliable predictions of tensile, fatigue, and fracture properties of metallic alloys. Under monotonic loading, finite element analyses and experiments were employed to characterize the elastic–plastic transition and the onset of plastic instability. Digital Image Correlation (DIC) was integrated with SPT to provide full-field strain measurement, revealing a shift of peak plastic strain from the specimen centre to a characteristic radial location where localization leads to instability and cracking. Refined correlations for yield strength, ultimate tensile strength, and ductility were established, reducing material dependency and improving predictive accuracy across diverse metallic alloys.

For cyclic loading, termed Small Punch Fatigue (SPF), progressive strain accumulation closely resembles uniaxial ratcheting fatigue behaviour. Systematic tests on SS 316LN and P91 steels enabled development of correlations between SPF and ratcheting fatigue, enabling fatigue life prediction directly from SPF data. Finally, notched SPT specimens were explored using 3D-DIC and FE simulations; strain localization at ~0.5–0.6 mm from the specimen centre was identified as the crack initiation site. A linear correlation between notch mouth opening displacement at instability and crack tip opening displacement from standard fracture tests demonstrates the potential of notched SPT for fracture toughness estimation.

The challenges in SPT arise from its complex multiaxial stress state and indirect property extraction. A transition from empirical correlations to more generalized relationships is expected to reduce uncertainty in translating results into conventional tensile, fatigue, and fracture properties.

Keywords: Small punch test, Deformation, Mechanical properties, Digital image correlation, Ratcheting

EXPLORING THE IRRADIATION RESPONSE OF MULTI-PRINCIPAL ELEMENT ALLOYS: INSIGHTS FROM PROTON-INDUCED DEFECT DYNAMICS AND RECOVERY

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ABSTRACT

The development of next-generation nuclear reactors hinges on structural materials capable of maintaining mechanical integrity under intense radiation flux. Multi-Principal Element Alloys (MPEAs) are hypothesized to offer superior radiation resistance compared to traditional austenitic stainless steels due to their inherent chemical complexity. The pronounced lattice distortion in MPEAs is expected to create a continuous landscape of energy traps for point defects, which is thought to impede the long-range migration of interstitials and vacancies, thereby enhancing defect recombination and reducing net radiation damage. This talk presents a systematic investigation into the proton-irradiation response of CoCrFeMnNi-based MPEA at room temperature and a reactor-relevant temperature of 300°C to evaluate whether these chemically complex alloys effectively suppress defect accumulation more efficiently than traditional steels. We explore the fundamental depth, dose, and temperature-dependent evolution of defects and correlate these microstructural features with nanoindentation profiles to elucidate the mechanisms driving irradiation hardening and altered deformation behavior. Finally, we discuss the recovery of mechanical properties via post-irradiation annealing, elucidating how the interplay between temperature and lattice distortion dictates the radiation tolerance of these next-generation alloys.

Open Challenges

- Long-term Stability
- Modelling irradiation response
- Scaling to Neutron Fluence

Keywords: High-entropy alloy (HEA), Dislocation loops, Voids, Nanoindentation, Irradiation hardening, Deformation mechanisms

References:

1. Chethan Konkati, N. Gayathri, P. Mukherjee, and Ankur Chauhan, "Proton-irradiation and post-irradiation annealing behavior of a CoCrFeMnNi-based multi-principal element alloy", Materials Science and Engineering: A, Vol. 945, 148968, 2025.

PHYSICS-BASED CONSTITUTIVE FRAMEWORK FOR α-ZR ALLOYS DEFORMED AT LOW TO WARM TEMPERATURES AND ACROSS QUASI-STATIC TO DYNAMIC STRAIN RATES

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ABSTRACT

Zircaloy-4 (an α-Zr alloy) is used as a fuel clad material in pressurised heavy water reactors. For accident case scenarios and advanced processing techniques, it is desirable to understand the deformation behaviour of this across a wide range of strain rates and temperatures. α-Zr alloys are anisotropic and depending on their orientation, will activate either prismatic <a> slip, pyramidal <c+a> slip or twins. The occurrence of twinning results in a sigmoidal stress-strain curve with a significant increase in work-hardening in the strain range where twinning occurs. Here a framework for a physics-based constitutive equation using the concept of thermally activated deformation applicable to Zircaloy-4 will be discussed. This constitutive model will be for a wide range of strain rates (from 10-3 to 103 s-1) and temperatures (from 25 to 500 °C), and will incorporate slip, twinning, and viscous drag (present at high strain rates).

Keywords: IN718, low cycle fatigue, stress softening, precipitate shearing, crystal plasticity

ELECTRONIC-STRUCTURE GOVERNED STRENGTHENING IN FACE-CENTERED CUBIC HIGH-ENTROPY ALLOYS: A UNIFIED FRAMEWORK FOR SOLID-SOLUTION AND GRAIN SIZE STRENGTHENING MECHANISMS

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ABSTRACT

It has been established that the presence of solute atoms of different atomic size creates a local stress field, or lattice distortion that interact with the dislocation stress field. In concentrated and high-entropy alloys (HEAs), a consequence of this stochastic distribution of alloying elements is that, dislocations must overcome an extra energy barrier, thus causing an increase in yield strength (YS). Varvenne et al [Acta Materialia, 118 (2016)] have derived a mechanistic model that accounts for the statistics of the solute-dislocation interactions highlighting the importance of lattice distortion arising due to the misfit volume among various solutes.

However, our current study shows that the conventional misfit volume parameter (δ) is insufficient for consistently predicting strengthening across Ni-based binary alloys and Ni–Co–Cr–Fe–Mn HEAs. Instead, charge-transfer-driven electronic interactions, quantified through the mean d-orbital energy mismatch (Md), are found to govern strengthening. A strong positive correlation is established between Md and solid-solution strength. This framework resolves anomalies such as the relatively low strength of Ni–20%Mo despite its highest δ (~5.68%). In contrast, alloys such as NiCoV exhibit highest strength with moderate δ (~3.65%) but larger Md (~0.376 eV). Alloys with similar Md values, irrespective of compositional complexity, display comparable strength and deformation behavior. That is, equalization of strength with the physical parameter, Md is shown for the first time. Grain-size strengthening follows a similar trend, with the Hall–Petch coefficient (kHP) scaling with both alloy strength and Md. The derived critical shear stress (τ_c) is consistent with the critical resolved shear stress (CRSS) obtained from single-crystal deformation, indicating a common electronic origin. These results establish Md as a unifying descriptor linking electronic structure with dislocation-mediated strengthening. The current findings demonstrate that neither solid-solution nor grain-size strengthening is inherently dependent on compositional complexity, providing a simplified framework for designing high-strength alloys with minimal alloying.

While δ captures long-range elastic strain fields arising from atomic size (volume) mismatch, Md reflects short-range electronic interactions that influence dislocation core energetics. The relationship between the electronic descriptor Md and the lattice distortion-based parameter, δ remains unresolved and represents a key open question in alloy strengthening. Furthermore, the present findings open further discussions on whether HEAs provide any added advantage compared to conventional alloys.

Keywords: d-orbital energy level, misfit volume parameter, solid-solution strengthening, high-entropy alloys

Keywords: IN718, low cycle fatigue, stress softening, precipitate shearing, crystal plasticity

CREEP OF ADDITIVELY MANUFACTURED NI-BASE SUPERALLOYS

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ABSTRACT

Additive manufacturing (AM) of Ni-base superalloys for gas turbine applications is gaining significant attention due to the design flexibility and processing advantages it offers over conventional routes. However, a thorough understanding of the creep behaviour of AM Ni-base superalloys has not been adequately addressed in the literature. Our work on creep of IN625 (solid-solution-strengthened), IN718 (γ''-strengthened), and IN939 (γ'-strengthened) suggests anisotropic creep behaviour, which can consequently affect their reliability in critical aerospace applications.

Creep behaviour of AM superalloys is intrinsically governed by underlying microstructural attributes inherited from various processing stages, particularly crystallographic texture, grain morphology, and segregation-driven precipitate evolution. The interplay among these attributes dictates the anisotropic response and damage mechanisms at elevated temperatures. However, establishing a unified understanding remains challenging, as the complex interplay between process-induced microstructural heterogeneity and mechanical behaviour remains unresolved. Bridging this gap is critical to developing reliable structure–property correlations to harness the full potential of AM superalloys.

Keywords: creep; additive manufacturing; laser powder bed fusion; anisotropy

HIGH-TEMPERATURE FATIGUE CRACK GROWTH BEHAVIOR OF STRUCTURAL MATERIALS: MECHANISTIC UNDERSTANDING AND EXPERIMENTAL ANALYSIS

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ABSTRACT

High-temperature fatigue crack growth (FCG) behavior of structural materials is governed by the complex interaction of cyclic loading, time-dependent deformation and environmental interactions, resulting in significant deviations from conventional room-temperature crack growth response. This study presents a mechanistic and experimental analysis of FCG behavior at elevated temperatures in engineering materials used in demanding high-temperature applications. Crack propagation at elevated temperatures is influenced by thermally activated mechanisms including diffusion, thermal ageing, oxidation, creep deformation, dislocation restructuring, recrystallization and microstructural degradation, along with thermal stresses and surface deterioration such as corrosion-induced pitting. These processes accelerate crack tip damage, promote grain boundary weakening and transitions in fracture modes. To take care of such deviations, high temperature FCG behavior needs to be described using two intrinsic driving forces: the cyclic stress intensity factor range (ΔK) and the maximum stress intensity factor (K_{max}), without invoking crack closure concepts. Crack propagation occurs when both cyclic and static thresholds are satisfied, where ΔK_{th} is associated with cyclic plasticity and K_{max}^* governs crack tip bond rupture. With increasing temperature, the contribution of time-dependent damage becomes more significant, leading to a dominant influence of K_{max}. Environmental effects further influence crack growth behavior, leading to oxidation-assisted cracking and transitions from transgranular to intergranular fracture, particularly in the near-threshold regime. In certain advanced alloys, a crossover behavior is observed, where higher crack growth rates in the Paris regime correspond to increased resistance in the near-threshold region due to environmentally driven fracture mode transitions. Accurate characterization of FCG behavior at elevated temperatures requires advanced experimental methodologies. In particular, in-situ crack monitoring techniques such as the direct current potential drop (DCPD) method are required for reliable crack length measurement, as conventional crack opening displacement (COD) gauges are limited due to thermal instability and measurement constraints under high-temperature conditions. The integration of mechanistic understanding with experimental observations provides a robust framework for interpreting high-temperature FCG behavior and improving predictive capability. Key findings from FCG studies of Alloy 617M at elevated temperatures are presented.

Keywords: Fatigue crack growth (FCG); Stress intensity factor range (ΔK); Threshold stress intensity factor range (ΔK_{th}); Direct current potential drop (DCPD); Crack opening displacement (COD); Alloy 617M.

A MULTISCALE FRAMEWORK FOR DEFORMATION IN DEFECT-RICH MATERIALS: BRIDGING CPFE AND ATOMISTIC SIMULATIONS

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ABSTRACT

Understanding deformation mechanisms in irradiated materials remains a central challenge in materials science, due to the combined effects of complex defect populations and severe experimental constraints. In neutron-irradiated materials such as tungsten, available samples are often limited in size and highly radioactive, restricting conventional mechanical testing and necessitating reliance on small-scale experiments such as nanoindentation. However, even these experiments present interpretation challenges: for example, strain-rate-dependent indentation responses are often convoluted with variations in penetration depth, making it difficult to isolate underlying mechanisms.

In this talk, we present a computational framework based on crystal plasticity finite element (CPFE) modeling that enables controlled interrogation of deformation mechanisms under such constraints. The model is first calibrated against nanoindentation experiments performed at a reference strain rate for both unirradiated and neutron-irradiated tungsten. A key pedagogical component of the framework is the incorporation of strain-rate sensitivity through a thermally activated slip law derived from a Helmholtz free energy formulation. The calibrated model is then used as a virtual laboratory to decouple the effects of strain rate and indentation depth, achieving quantitative agreement with experimental load–displacement response, surface pile-up, and lattice rotation fields measured via high-resolution EBSD.

To incorporate irradiation-induced defect physics, we integrate insights from molecular dynamics (MD) simulations and microscopy. Defect populations characterized via TEM are translated into effective resistance to dislocation motion using interaction strengths obtained from MD simulations for voids and precipitates, while analytical estimates are employed for larger defect clusters such as dislocation loops. This establishes a pathway for transferring atomistic information into continuum-scale deformation models.

However, these results also expose a fundamental limitation: the strength of defect populations cannot be uniquely defined by deterministic parameters due to the vast variability in defect size, orientation, spatial distribution, and interaction history. To demonstrate this issue, the talk will also showcase MD simulations of dislocation–loop interactions in tungsten illustrating a strong sensitivity of interaction strength to these factors, highlighting the inadequacy of current approaches that rely on simplified representations.

The talk will conclude by outlining an open challenge in the field: the development of statistically representative, computationally tractable descriptions of defect-mediated strengthening that can be systematically integrated into continuum models such as CPFE. Addressing this challenge is essential for enabling predictive, physics-based simulations of deformation in complex, defected materials.

Keywords: Crystal Plasticity Finite Element Method (CPFE); Molecular Dynamics (MD); Irradiation Damage; Dislocation–Defect Interactions; Defect Statistics / Statistical Strength

PERSPECTIVES ON THE MECHANICAL BEHAVIOUR OF MATERIALS

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