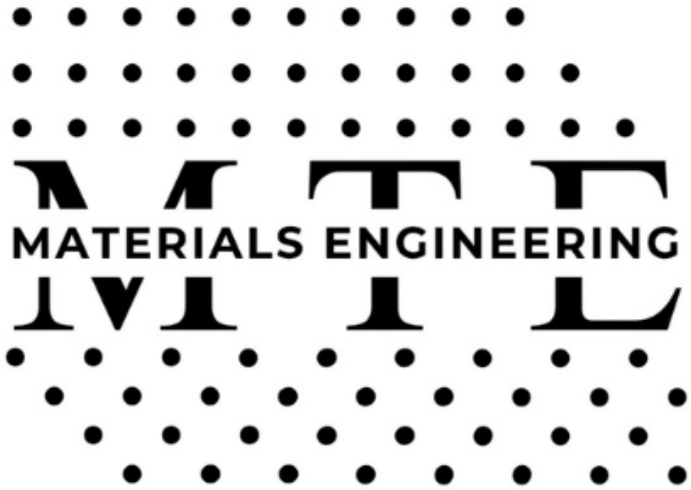
38th Annual Student Symposium



Department of Materials Engineering, Indian Institute of Science, Bangalore-560012, India

Book of Abstracts

Feb 20th-21st, 2025

Contents

38th Annual Student Symposium – Welcome Letter

Prof. Satyam Suwas

Chairman, Department of Materials Engineering, Indian Institute of Science, Bangalore

Dear Participants,

As we step into the 2025 academic session, we find ourselves at the threshold of a significant milestone in the history of the Department of Materials Engineering at the Indian Institute of Science (IISc), Bangalore. This year, we proudly host the **38th Annual Student Symposium on Metallurgical and Materials Research**, a testament to the enduring legacy and evolving dynamism of our department. Since its inception on the cusp of India's independence and its transformative journey from the Department of Metallurgy to the Department of Materials Engineering, we have been at the forefront of the materials revolution in India.

Our alumni have emerged as leaders across diverse sectors, shaping technologies in iron & steel, nuclear materials, biomaterials, and beyond, spanning the macro scale of large reactors to the precision of nanodevices. This enduring success is rooted in our commitment to excellence and innovation, reflecting the broad spectrum of our engagement with engineering materials. As we navigate through our journey, the renaming of our department in its diamond jubilee year symbolized not just a change in name, but a renewed pledge to advance the frontiers of materials engineering.

The Annual Student Symposium has always been a reflection of our department's vitality, driven by the relentless spirit of our students. It was their vision that brought this event to life 38 years ago, establishing a tradition of excellence and continuous learning that has grown year after year. This symposium is not just an opportunity to display our organizational capabilities but also a platform to benchmark our research achievements against global standards. The compilation of abstracts showcased here mirrors the current research landscape within our department, highlighting the innovative work of our students and faculty.

As we gather to celebrate this occasion, we extend a heartfelt welcome to our esteemed alumni, whose achievements and contributions continue to inspire us. Your presence serves as a bridge connecting our rich past with the promising future ahead.

On behalf of my colleagues and our vibrant student community, it is my honor to invite you to

join us from February 20 to 21, 2025, for a confluence of minds and ideas that promises to shape the future of materials engineering. Your participation, feedback, and insights are invaluable as we strive to chart a path forward, buoyed by optimism and the endless possibilities that lie ahead.

In anticipation of your presence and contributions, let us come together to celebrate the spirit of inquiry and innovation that defines our department.

Prof. Satyam Suwas

Chairman

Department of Materials Engineering

Indian Institute of Science, Bangalore

Foreword from the Organizers

Organizing Committee

38th Annual Student Symposium, Department of Materials Engineering, IISc Bangalore

It is with great enthusiasm and a deep sense of responsibility that we embark on the organization of the **38th Annual Student Symposium on Metallurgical and Materials Research** at the Department of Materials Engineering, IISc Bangalore. Scheduled for **February 20th to 21st, 2025**, this event is not merely a continuation of a revered tradition, but also a testament to the enduring spirit of innovation and inquiry that defines our department.

The Student Symposium has long been a pivotal event in our academic calendar, fostering a vibrant exchange of ideas among students and faculty alike. It provides a stage for budding researchers to showcase their work, encouraging discussions that transcend conventional boundaries within metallurgy and materials science. This year, as we gather to celebrate past achievements and set our sights on new frontiers, the symposium holds special significance. It underscores the department's ongoing commitment to excellence, echoing our collective aspirations for the future.

The overwhelming response from the student community underscores the dynamic academic environment that our department nurtures. The *Abstract Booklet*, which lies at the heart of the symposium, captures the breadth and depth of research conducted by our students. From advanced materials processing to pioneering applications in nanotechnology and biomaterials, these abstracts offer a glimpse into the future of materials engineering.

In line with the evolving landscape of research and industry, this year's symposium features a **special session on entrepreneurship in Metallurgy and Materials Engineering**. This initiative seeks to bridge the gap between academic research and practical applications, inspiring students to explore the entrepreneurial potential of their work. We are honored to have distinguished faculty and successful entrepreneurs share their experiences, thus enriching the symposium experience.

We extend our heartfelt gratitude to **Prof. Satyam Suwas**, our esteemed Chairman, for his unwavering support and guidance. His visionary leadership not only steers our department toward excellence but also inspires us to reach greater heights. We also wish to thank our Faculty Advisor and all our faculty members for their invaluable contributions to making this event a

success.

Last but not least, we owe a special debt of gratitude to the student community. Your enthusiasm, creativity, and diligent efforts are the lifeblood of this symposium. From the innovative research abstracts to the artistic design of the logo and cover page of the Abstract Booklet, your contributions exemplify the spirit of collaboration and excellence that our department upholds.

As we prepare for the **38th Annual Student Symposium**, we reflect on the legacy we carry forward and the new chapters we have yet to write. May this symposium stand as a celebration of our past accomplishments and a guiding light for our future endeavors.

On behalf of the organizing committee, we warmly invite you to join us in this celebration of knowledge, innovation, and community. Together, let us embark on a journey of discovery that not only honors our department's storied past but also paves the way for a future of limitless possibilities.

Organizing Committee

38th Annual Student Symposium

Department of Materials Engineering

IISc Bangalore

Committees

General Chairs

Prof. Satyam Suwas

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Prof. Ankur Chauhan

Student Committee

Ashitha D Pattabi

Sistla Sri Venkata Sarath Chandra

Nipun Jain

Chirantandip Mahanta

Schedule

Day 1 - 20th February 2025

Time	Talks/Presentations	
9:30 am - 9:45 am	**Opening Ceremony & Welcome Address by the Chair**	
9:45 am - 10:45 am	**Keynote Speaker (Dr. S.V. Ramana Murty)**	
10:45 am - 11:00 am	High Tea	
	Oral Presentations	
	KI Vasu	**KPA**
11:00 am - 11:15 am	**Prasanth Soundappan**: Mechanism and mitigation of crack formation in laser-based directed energy deposition of γ-TiAl powder	**Balpartap Singh**: Spacer Cation Rigidity Dictates Structural and Excited State Dynamics in 2D Halide Perovskites
11:15 am - 11:30 am	**Sourav Maji**: Impact of Ge as an alloying addition on microstructure and high-temperature mechanical properties of 2nd Generation TiAl alloy	**Mohammed Hadhi PP**: Wafer-Scale Solution-Processed 2D-TMD Transistors and Circuits Enabled by Single-Flake Transport
11:30 am - 11:45 am	**Chethan Konkati**: Proton irradiation effects on multi-principal element alloy	**Manvendra Singh**: Low-temperature fabricated solution-processed diodes for wireless paper electronics

11:45 am - 12:00 pm	**Raineesh Kp Babu**: Room Temperature Creep in Ti6242	**Durgesh Borkar**: Modulating Band Offset through Interface Engineering of Cu_2SnSe_3-Based Heterojunctions for Efficient Charge Separation and Collection
12:00 pm - 12:15 pm	**Sita Choudhary**: Effect of process parameters and heat treatment on structure and mechanical properties of directed energy deposited Ti6242	**Pooja Punetha**: Nature of morphotropic phase boundary in the lead-free piezoelectric systems $K_{1/2}Bi_{1/2}(M_{1/3}Nb_{2/3})xTi_{1-x}O_3$: M = Mg, Zn
12:15 pm - 12:30 pm	**Sunando Banerjee**: Effect of texture, grain boundary constitution, and molybdenum partitioning on corrosion and hydrogen permeation behavior of pulse electrodeposited Ni-Mo coatings.	**Amarakonda Chandana Siri**: Screen printed micro-supercapacitors on paper with additive-free 1T MoS_2 ink for sustainable energy solutions
12:30 pm - 12:45 pm	**Vamsi Krishna Paki**: Effect of reduction per pass during high-temperature rolling of Mg-1wt%Gd alloy on texture, mechanical, and corrosion properties	**Kaushal Tiwari**: Development of tunable ferroelectric thin films for the bandpass filters in the satellite systems
12:45 pm - 1:00 pm	**Divya Nalajala**: Towards Single Crystal Growth in CMSX-4	**Getaw Abebe Tina**: Simultaneous enhancement of d_{33} and depolarization temperature of the Superalloy Builds Using Laser Directed Energy Deposition
1:00 pm - 2:00 pm	Lunch Break	

2:00 pm - 2:50 pm	**Invited Talk (Mr. Sankarappa Prasad)**	
	Oral Presentations	
2:45 pm - 3:00 pm	**Abhinav Chandraker**: Experimentally validated and empirically compared machine learning approach for predicting yield strength of additively manufactured multi-principal element alloys	**Vimalkumar S**: Upcycling post-consumer recyclate of Polyamide 66 by controlling chain scission and crosslinking density
3:00 pm - 3:15 pm	**Shiba Sankar Dash**: DFT study of hydrogen interstitial solute interaction with dislocations in nickel	**Samvidha Das**: Design and Investigation of MIL-100 (Fe) Metal-Organic Frameworks for Controlled Drug Delivery
3:15 pm - 3:30 pm	**Subramanian R S**: Exploring the state-of-the-art in quantum computing for computational materials science	**Bharath Sriram Gugulothu**: 3D Bioprinted Metastatic Niches of Triple Negative Breast Cancer for Drug Screening
3:30 pm - 3:45 pm	**Swapnil Bhure**: A Roadmap for Producing Single-Crystal Ni-Based Superalloy Components Using Laser-Directed Energy Deposition	**Indranil Dey**: Recycling Reinvented: Converting PET Bottle Waste into 3D printable PCR Polypropylene Vitrimers for a Sustainable Future

3:45 pm - 4:00 pm	**Ankur Srivastava**: Diffusion analysis in binary and ternary Ni-based alloys following Experimental, Density Functional Theory (DFT) and Physics-informed neural network numerical inverse method (PINN)	**Nipun Jain**: Engineering 3D bio-printed Lung-on-a-Dish platform to investigate Pulmonary Fibrosis
4:05 pm - 4:40 pm	**Invited talk (Prof. P. Rajamali)**	
4:40 pm - 4:50 pm	Tea Break	
4:50 pm - 5:45 pm	**Poster and materialography judging session**	

Day 2– 21st February 2025

Time	Talks/Presentations
9:30 am - 10:45 am	**Keynote Speaker (Prof. Raman Singh)**
10:45 am - 11:00 am	High Tea
11:00 am - 12:10 pm	**Industry – Academia Panel Discussion (Dr. Prince Singh, Dr. Manjini S, Dr. T Ramprabhu)**
12:10 pm - 12:45 pm	**Springer talk**
12:45 pm - 2:00 pm	Lunch Break

2:00 pm - 2:35 pm	**Invited Talk (Dr. Manjini S)**	
	KI Vasu Auditorium	**KPA Auditorium**
2:45 pm - 3:00 pm	**Suraj Kumar**: Development of High-temperature DIC (up to 1800 °C) for strain measurements	**Arup Kumar Mandal**: Understanding Complex Magnetic Interfacial Exchange Interactions and Magnetic Tunnel Resistance Behaviour of Epitaxially Grown $SrRuO_3/BiFeO_3/La_{0.7}Sr_{0.3}MnO_3$ Heterostructure
3:00 pm - 3:15 pm	**Shubham Sisodia**: Enhancing fatigue resistance of Cr-Mn-Fe-Co-Ni system by varying composition and sigma-phase assisted grain-size reduction	**Satyam Jena**: Harnessing Excited-State Charge Transfer for the Activation of Dark Triplet Excitons and Phosphorescence in Hybrid Organic-Inorganic 2D Perovskite
3:15 pm - 3:30 pm	**Darshan C**: Creep and Stress Relaxation in Thin Films: Experiments, Modelling, and Materials Science-Based Insights for Reliability Improvement	**Shikha Akshay Joshi**: Fabrication and analysis of oxide-based ferroelectric gated transistors using the Inkjet-Printing technique
3:30 pm - 3:45 pm	**Kalyan D**: Development of High strength and High Conductive Cu-based alloys	**Bappa Daa**: Semi solid TIG-based Additive manufacturing of Al-15Mg_2Si-4.5Si-0.01Sr0.015B composite
3:45 pm - 4:00 pm	**Bavithra M**: Enhanced Corrosion Resistance of AZ31 Magnesium Alloy through LDH Coating and 8-Hydroxyquinoline Intercalation	**Animesh Mandal**: Influence of Transition Metal Doping on the Exciton Dynamics in All-Inorganic Metal Halide Perovskite

4:00 pm - 4:15 pm	**Gudeta Jafo Muleta**: Simultaneous increase of d_{33} and Curie point of PZT by dilute rare earth doping: the phenomenon and the mechanism	
4:15 pm - 4:30 pm	Tea Break	
4:30 pm - 5:30 pm	**Closing Ceremony**	
7:00 pm - 9:00 pm	Dinner	

Invited Talks

Polymeric Materials: Benefiting from Adopting Conformity Assessment Practices for Safety, Sustainability, and Performance

Prasad Shankarappa

UL's Engineered Materials Division

Conformity assessment involves a set of processes that validate compliance with a standard or a set of specific requirements for a product, service, or system. The primary forms of conformity assessment include testing, certification, and inspection.

The adoption of these best practices is vital for the global polymeric industry, as polymeric materials serve critical functions in various engineering applications, including aerospace, defense, automotive, wind energy, electrical, and electronics. These materials must continuously demonstrate compliance with stringent technical specifications and standards.

This talk examines the benefits of adopting conformity assessment practices through a use case scenario of UL's Yellow Card Program for Plastics Pre-selection, specifically for plastic materials used in electrical and electronic devices and appliances. Compliance testing of polymeric materials to evaluate and report their performance characteristics, along with inspection and assessment methodologies at material manufacturing sites, will also be discussed.

Biography: Prasad Shankarappa is a Principal Engineer under UL's Engineered Materials division in the Testing-Inspection-Certification (TIC) business unit. As a Principal Engineer, he is responsible for UL Safety Standards related to Plastics Certification Testing and Long-Term Property Evaluations of plastic compounds.

Prasad holds a Bachelor's Degree in Polymer Science and Technology from SJCE, Mysore, and a double Master's Degree in Materials Science and Engineering from Sweden and France. With 21 years of experience at UL, he has contributed significantly to Conformity Assessment, Standards Development, Testing, and Safety Certification of Plastics and Color/Additive Concentrates.

Keywords: Conformity Assessment, Polymer Testing, UL Yellow Card, Plastics Certification, Safety Standards.

Metal-Free Emitters for Organic Light Emitting Diodes

P. Rajamalli

Department of Organic Chemistry, Indian Institute of Science (IISc), Bangalore, India

Ultra-deep blue fluorescent emitters with CIEy < 0.08 are still in demand for achieving vibrant full-color displays. In this work, we have designed and synthesized xanthene-anthracene-based PhAn-Xn, where xanthene and anthracene are linked by an orthogonal phenyl bridge, effectively preventing aggregation-caused quenching (ACQ). PhAn-Xn exhibits emission maxima at 430 nm, full width at half maxima (FWHM) of 48 nm, and a prompt lifetime ($\ddot{I}\check{D}_P$) of 0.7 ns.

The non-doped OLED device based on PhAn-Xn shows electroluminescence (EL) maxima at 432 nm, achieving a maximum external quantum efficiency (EQE_{max}) of 4.2% with Commission Internationale de L'ÃĽclairage (CIE) coordinates of (0.16, 0.06) at 8V, and a maximum luminance (L_{max}) of 4,110 cd m^{-2}. The device maintains an EQE of 4.0% at 1,000 cd m^{-2}, retaining 95% of the maximum efficiency.

Additionally, PhAn-Xn, which demonstrates superior charge transport properties compared to the commonly used blue host DPEPO, is employed as a host material in OLED devices, incorporating the well-known blue dopant 4,'âĂŹ-Bis(9-ethyl-3-carbazovinylene)-1,1'-biphenyl (BCzVBi). The doped device exhibits EL maxima at 455 nm, consistent with the photoluminescence (PL) spectra. It achieves an EQE_{max} of 6.5% along with a high brightness of 41,557 cd m^{-2}. The device retains 98% of its maximum efficiency at 1,000 cd m^{-2}, maintaining an EQE of 6.4%. These results highlight the multifunctionality of PhAn-Xn, serving as both an emitter and a host for deep blue OLEDs.

Biography: Dr. P. Rajamalli obtained her Ph.D. in Physical Organic Chemistry from the Department of Chemistry, IIT Madras, in 2012. She subsequently undertook a post-doctoral position at National Tsing Hua University (NTHU), Taiwan, with Prof. Chien-Hong Cheng (2012-2016). Following this, she received the prestigious Marie Curie Postdoctoral Fellowship and worked with Prof. Eli Zysman-Colman at the University of St Andrews, UK (2016-2019). Dr. Rajamalli joined IISc Bangalore as an Assistant Professor in 2019, where her research focuses on developing emitting materials for organic light-emitting diodes (OLEDs), including TADF (Thermally Activated Delayed Fluorescence), MR-TADF (Multiple Resonance TADF) emitters,

carbon quantum dots, and dendrimer-based emitters for solution-processed OLEDs. Her group also works on designing host and electron-transporting materials for highly stable devices. The research covers the entire OLED material development pipeline, from molecular design and synthesis to photophysical studies and device fabrication.

Keywords: OLED, Deep Blue Emission, TADF, ACQ Prevention, Organic Semiconductors.

Industry –Academia Panel Discussion

Reliability Engineering at Bosch

Prince Singh

Bosch Global Software Technologies

Reliability engineering plays a crucial role in product development by ensuring durability, performance, and safety. This talk will discuss the principles of reliability engineering in product design and their relevance to materials engineers. Additionally, insights into the implementation of reliability engineering at Bosch will be provided.

Biography: Dr. Prince Singh is a mechanical engineer and reliability specialist with a strong background in materials engineering, mechanical design, and system reliability. With over a decade of experience spanning academia and industry, he has made significant contributions to engineering design and reliability analysis.

Dr. Singh earned his B.Tech in Mechanical Engineering from Harcourt Butler Technical University (2005-2009) before pursuing an M.E. in Materials Engineering from IISc Bangalore (2009-2011). He then worked as a Design Engineer at Tata Hitachi Construction Machinery Limited (2011-2014), where he gained hands-on experience in mechanical systems and product development. Driven by a passion for research and innovation, he pursued a Ph.D. in Mechanical Engineering at Carnegie Mellon University, Pittsburgh (2014-2019), focusing on advanced mechanical systems, materials science, and reliability engineering.

Since 2020, Dr. Singh has been working as a Reliability Specialist at Bosch Global Software Technologies, applying his expertise in predictive maintenance, failure analysis, and system optimization to enhance product durability and efficiency.

Keywords: Reliability Engineering, Failure Analysis, Product Development, Predictive Maintenance.

Comparative Assessment of Materials Engineering Research at IISc and its Relevance to the Indian Military Aerospace Program

T. Ram Prabhu

Defence Research and Development Organization (DRDO), Government of India

A short review of materials engineering theses from the Indian Institute of Science (IISc), spanning the period 2001-2024, has been undertaken, with a particular focus on aerospace alloys. Key findings from this review are juxtaposed against the performance characteristics of established "workhorse "alloys currently employed in the Indian military aircraft program.
A subsequent discussion will explore subjective observations and analytical insights derived from this comparative assessment, emphasizing the alignment of academic research with practical aerospace applications and identifying potential gaps and opportunities for future development.

Biography: Dr. T. Ram Prabhu is a distinguished scientist and academician with over 15 years of research experience in engineering design and materials science. He currently serves as a Scientist 'E 'and Joint Director at DRDO, Government of India, where he has made significant contributions to metal additive manufacturing, aerospace materials, and defense technologies.
Dr. Prabhu holds a Ph.D. in Engineering Design from IIT Madras, an M.E. in Materials from IISc Bangalore, and a B.Tech in Metallurgy from NIT Trichy, along with additional qualifications in applied statistics and finance management. His career spans both academia and industry, including roles at ESSAR Steel Ltd. and Smart Analyst Pvt. Ltd., before joining DRDO in 2009. Dr. Prabhu continues to be a driving force in India's defense technology sector, bridging the gap between research, innovation, and industry implementation.

Keywords: Aerospace Alloys, IISc Research, Military Aircraft Materials, Metal Additive Manufacturing, Defense Technologies.

Oral Abstracts

Design and Investigation of MIL-100 (Fe) Metal-Organic Frameworks for Controlled Drug Delivery

Samvidha Das, Ashok M. Raichur

Department of Materials Engineering, Indian Institute of Science Bangalore

Cancer-related deaths crossed 9.7 million in 2022 and are predicted to increase beyond 35 million by 2050. Nanomedicines, such as Nano-metal-organic frameworks (nMOFs), possess superior drug-loading capacities, attributed to their elevated surface area and pore volume. However, their direct biomedical application is limited owing to their irregular shape, heterogeneous morphology, and large size. Hence, to address this lacuna, we devised a synthesis method (one-pot, room-temperature synthesis method) to regulate the size and morphology of MIL-100 (Fe) nMOF, aiming for controlled biological responses under Tumor Microenvironment (TME), targeted and controlled drug release. In this study, spherical homogenous nMOFs were obtained with FCC crystal structure and 160 nm diameter. Further, the in vitro analysis of the as-designed nanomedicine over breast carcinoma cells (MCF-7) was found to be inherently anti-cancerous via excessive Reactive Oxygen Species (ROS) generation, augmented to the internalization of MIL-100 (Fe) under TME. The therapeutic efficacy of the developed system was studied using Camptothecin (CPT), an FDA-approved anticancer drug, that demonstrated high drug loading (drug loading capacity of 81.5%) and stimuli-responsive release profile (>75% within 24 hours in acidic pH). The developed synthesis method overcomes the major drawback of MIL-100 (Fe), i.e., size irregularity and morphology heterogeneity, which limits its biomedical applications. This intrinsic anti-cancerous property of MIL-100 (Fe) along with pH-dependent drug release behaviour forms a synergistic platform to combat breast cancer.

Keywords: Nano-metal-organic frameworks (nMOFs), MIL-100 (Fe), Targeted drug delivery, Cancer therapy.

Effect of process parameters and heat treatment on structure and mechanical properties of directed energy deposited Ti6242

Sita Choudhary[1], Prasanth Soundappan[2], Debtanay Das[1], Satyam Suwas[1]

[1] Department of Materials Engineering, Indian Institute of Science Bangalore-560012, INDIA

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As printed Ti6242 has good strength due to non-equilibrium refined microstructure but ductility is very low ($< 10\%$). Therefore, in this study, we aim to investigate the effect of post-processing heat-treatment on mechanical properties of DED printed near-alpha Ti6242 alloy. Microstructural and structural characterization was done using Optical, SEM, and XRD. X-ray computed tomography was done to analyze the porosity distribution in the as-printed condition. Post-processing cyclic heat-treatment was designed. Mechanical properties were analyzed for both as-printed and heat-treated conditions by uniaxial tensile test. The as-printed condition resulted in high yield strength of about 1350 MPa with the elongation of about 5%. Post-processing heat-treatment led to the formation of equilibrium alpha and beta phases, leading to improvement in the ductility at the expense of strength. Cyclic heat-treatment results in the formation of globular alpha and increased lath thickness. This study shows that with the design of a suitable heat-treatment, mechanical properties of the printed parts can be improved.

Keywords: DED, Heat-treatment, Microstructure, Mechanical Properties.

Modulating Band Offset through Interface Engineering of Cu_2SnSe_3-Based Heterojunctions for Efficient Charge Separation and Collection

Durgesh R. Borkar, Sachin R. Rondiya

Department of Materials Engineering, Indian Institute of Science, Bangalore 560012, India

Cu_2SnSe_3 (CTSe) shows promise due to its wide solar absorption and tunable band gap, though low efficiency caused by interface recombination and crystallinity issues remains a challenge. In this study, we demonstrate a systematic and facile synthesis method for CTSe nanoparticles (NPs), accompanied by an in-depth analysis of their nucleation and growth mechanisms. A comprehensive experimental and theoretical investigation was conducted to explore the structural, morphological, compositional, optoelectronic, and band alignment properties of p-type CTSe NPs as a solar absorber, along with n-type CdSe and ZnSe NPs as buffer layers.

Additionally, the band edge positions of the synthesized NPs were estimated using cyclic voltammetry (CV), ultraviolet photoelectron spectroscopy (UPS), and density functional theory (DFT), enabling the modulation of band offsets through interface engineering. Our investigation revealed a staggered type-II band alignment at the CTSe/CdSe heterojunction, characterized by a minimal conduction band offset (CBO) of 0.06 eV. The findings from CV and UPS measurements supported by ab initio density functional theory-based calculations suggest effective charge carrier separation and transport at the interface. The CTSe/CdSe heterojunction exhibited Schottky I-V characteristics, demonstrating a current of 1mA in dark conditions. These findings highlight the potential of CTSe NPs as an efficient absorber material in thin-film solar cells, providing a foundation for overcoming interface recombination losses and enhancing device performance.

Keywords: Cu_2SnSe_3, Band Offset, Interface Engineering, Charge Separation, Solar Cells.

Creep and Stress Relaxation in Thin Films: Experiments, Modelling, and Materials Science-Based Insights for Reliability Improvement

Darshan C, Praveen Kumar

Department of Materials Engineering, Indian Institute of Science, Bangalore, 560012, India

Materials used in microelectronics and integrated circuits can be subjected to temperatures as high as 400°C during their operation. Since these thin films are primarily deposited on silicon (Si) substrates and due to the significant difference in the thermal expansion coefficients of Si and the metallic films, the films develop substantial stresses ranging from several hundreds of Mega-pascals to Giga-pascals. Under these conditions, the films tend to relax their stresses through creep, formation of hillocks, interfacial sliding, and fracture, which deteriorates the life of the thin film devices. Hence, comprehending these stress relaxation mechanisms and trying to constrain them becomes essential.

In this study, we used a custom-built laser curvature setup to perform stress relaxation on Aluminum thin films of approximately 200 nm thickness with temperatures ranging from 250 to 400°C. If stress relaxation tests are performed on Al films deposited directly on the Si substrates, the relaxation observed would be a cumulative effect of creep, hillocks, and interfacial sliding. However, as the primary objective of this study is to correlate creep and stress relaxation in Al films, a titanium nitride (TiN) interlayer and passivation layer of 20 nm each is deposited, such that the Al film is sandwiched between these two TiN layers. The interlayer of TiN reduces the relaxation due to interfacial sliding, whereas the top passivation layer of TiN reduces the relaxation due to the formation of hillocks. This ensured that most of the stress relaxation was due to creep. These results are then utilised to predict the dominant creep mechanisms at the above-mentioned temperature ranges. Further, these experimental results were backed by FEM simulations which showed good agreement with one another.

Keywords: Thin films, Creep, Stress relaxation, Hillocks.

Effect of Texture, Grain Boundary Constitution, and Molybdenum Partitioning on Corrosion and Hydrogen Permeation Behavior of Pulse Electrodeposited Ni-Mo Coatings

Sunando Banerjee, Akhand Pratap Singh, Chandan Srivastava

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The study examines the microstructural evolution, electrochemical corrosion, and hydrogen permeation in pulse electrodeposited Ni-Mo coatings with varying Mo contents (2, 4, 8, and 11 wt% Mo). Electrochemical impedance spectroscopy and potentiodynamic polarization measurements revealed an improvement in corrosion resistance at an optimum Mo content. The corrosion current density i_{corr} and polarization resistance R_p values obtained were 13.8 μA/cm^2 and 1745 Ωcm^2, respectively, for the pure Ni coating, while the i_{corr} and R_p values obtained were 1.7 μA/cm^2 and 5406 Ωcm^2, respectively, for the Ni-4wt% Mo coating. Further, increased Mo content beyond 4 wt% increased the corrosion rate. Nevertheless, the corrosion resistance of Ni-Mo coatings was found to be higher than the pure Ni coating.

Ni-Mo coatings contained relatively Mo-enriched clusters in a solid solution matrix. The highest corrosion resistance of the Ni-4wt% Mo coating was due to lower energy (001) and (111) textures, lower energy grain boundary constitution, and low coating strain. In the Ni-4wt% Mo coating, Mo-enriched Ni-Mo nanoclusters inhibited hydrogen passage by providing a tortuous path. In contrast, a high fraction of high-angle grain boundaries (compared to pure Ni coating) facilitated hydrogen permeation, leading to a similar extent of hydrogen permeation through pure Ni and Ni-4wt% Mo coatings.

Keywords: Ni-Mo coatings, Cluster, Texture, Hydrogen permeation.

Development of High-temperature DIC (up to 1800°C) for Strain Measurements

Suraj Kumar, Vikram Jayaram, Praveen Kumar

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The demand for high-speed vehicles (above Mach 5) and energy efficiency is motivating the development and testing of new high-temperature materials. One of the major challenges associated with high-temperature mechanical testing is strain measurement. Here, we have established a digital image correlation (DIC) technique that can measure strain up to 1800°C. Isothermal experiments are conducted on three high-temperature materials, Nb-C103, Cf/SiC, and β-NiAl, at temperatures up to 1800°C. The testing is performed in both air and inert environments.

The standard deviation in the strain at isothermal conditions is within 4×10^{-4}, which is well within the acceptable range. The coefficient of thermal expansion of Cf/SiC is measured and validated with literature. The speckle paint is stable enough to run long experiments, and the DIC system is flexible enough to be integrated with any mechanical testing system if the sample is accessible through a viewport.

Keywords: DIC, Strain measurement, High-temperature.

Spacer Cation Rigidity Dictates Structural and Excited State Dynamics in 2D Halide Perovskites

Balpartap Singh, Sachin R. Rondiya

Department of Materials Engineering, Indian Institute of Science, Bengaluru, India

The exploration of two-dimensional (2D) perovskites has garnered significant attention due to their outstanding optoelectronic properties, passivation capabilities, and moisture resistance. In this work, the aromatic spacer cations were selected upon consideration of (i) molecule rigidity, (ii) band energy levels, and (iii) the extent of non-covalent interactions. This allowed us to understand the impact of aromatic linker rigidity on the perovskite structure. Accordingly, we synthesized a novel spacer cation, 2,2'-bithiophene, with increased rigidity and possibly phonon modes compared to phenethylamine and thiophenethylamine. X-ray diffraction studies showed no phase transitions at cryogenic temperatures due to the restricted degree of freedom (rotation or tilting) caused by steric hindrance. Moreover, $\pi - \pi$ stacking interactions in thio- and bithiophene limit the degree of lattice expansion.

Room temperature photoluminescence (PL) showed efficient quenching in $BTEA^+$ due to the localization of charge carriers at the valence band, which was well supported by static DFT calculations. Furthermore, cryogenic PL studies showed a decreasing trend of exciton binding energies, i.e., almost 50% reduction in E_b for $BThEA_2PbI_4$ compared to PEA_2PbI_4, which holds great significance in optoelectronic applications. In contrast, exciton-phonon coupling strengths showed an opposite trend, indicating competition between exciton-phonon interactions and stability induced by rigid cations in determining the excited-state dynamics. To gain a deeper understanding of cation-octahedra interactions, we performed XPS, which showed a concurrent peak shift in Pb-4f and I-3d orbitals attributed to the increased electron cloud overlap between Pb and iodide atoms in the lattices. Finally, we discussed an inherent donor-acceptor complex formation controlling exciton dynamics. The current work provides a general framework for the screening of electroactive spacer cations, enabling efficient carrier transport in otherwise poor carrier conductor 2D perovskites.

Keywords: 2D Perovskites, $\pi - \pi$ interactions, Distortions, Exciton-phonon coupling.

Enhanced Corrosion Resistance of AZ31 Magnesium Alloy through LDH Coating and 8-Hydroxyquinoline Intercalation

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Magnesium (Mg) and its alloys have gained significant attention in industrial applications due to their high specific strength. However, their susceptibility to corrosion remains a major challenge. In this study, a Layered Double Hydroxide (LDH) coating was developed on AZ31 Mg alloy to enhance its corrosion resistance. Additionally, 8-Hydroxyquinoline (8HQ), an environmentally friendly corrosion inhibitor, was intercalated within the LDH structure to provide active protection.

The structural and morphological characteristics of LDH and 8HQ-LDH coatings were analyzed using X-ray diffraction (XRD) and scanning electron microscopy (SEM). Electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization tests were conducted to assess the corrosion behavior of the coated samples in 0.5 wt.% NaCl aqueous solution. The results demonstrate that LDH coating significantly improves the corrosion resistance of AZ31 Mg, while 8HQ intercalated LDH further enhances its corrosion resistance. This study highlights the potential of LDH-based smart coatings as an effective strategy for mitigating magnesium alloy corrosion in various applications.

Keywords: LDH coating, Magnesium alloy, Corrosion resistance, 8-Hydroxyquinoline.

Understanding Complex Magnetic Interfacial Exchange Interactions and Magnetic Tunnel Resistance Behaviour of Epitaxially Grown $SrRuO_3/BiFeO_3/La_{0.7}Sr_{0.3}MnO_3$ Heterostructure

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This study demonstrates complex magnetic exchange interactions in epitaxially grown $SrRuO_3/BiFeO_3/La_{0.7}Sr_{0.3}MnO_3$ by conventional magnetic and spectroscopic techniques. We have also demonstrated tunnel magnetoresistance behaviour of the same under different external magnetic field configurations. The modified exchange coupling between SRO and LSMO in the presence of BFO creates multiple resistance states in electron tunnelling.

Quantum mechanical tunnelling in ferromagnetic tunnel junctions characterized by tunnel magnetoresistance has great potential applications in spintronic devices. It is essential to understand magnetic exchange coupling and electronic band alignment at the ferromagnetic layers to tune electron tunnelling through the insulating barrier. Most conventional soft ferromagnetic metal-based tunnel junction devices exhibit two-state switching between high and low resistance, which can be explained by the triple-spin flip model. Here, we demonstrate tunnel magnetoresistance based on complex perovskite ferromagnetic and ferroelectric materials.

We successfully modified the magnetic exchange interaction between ferromagnetic layers ($SrRuO_3$ and $La_{0.7}Sr_{0.3}MnO_3$) through multiferroic $BiFeO_3$ and simultaneously created multiple resistance states for the first time. The conventional triple-spin flip model deviates in complex perovskite-based magnetic tunnel junctions and creates multiple resistance states, which can be beneficial for future neuromorphic computations.

This study also demonstrates the complex magnetic coupling between LSMO, BFO, and SRO and their magnetic tunnelling behaviour. Experimental results, including out-of-plane XRD analysis and magnetization measurements with varying BFO thickness, confirm the presence of antiferromagnetic coupling between LSMO and SRO. Tunnel resistance measurements further validate layer-wise switching of SRO along the applied field direction, resulting in multiple resistance states.

Keywords: Magnetic Tunnel Junctions, Exchange Coupling, Tunnel Magnetoresistance, Perovskite Heterostructures, Spintronics.

Recycling Reinvented: Converting PET Bottle Waste into 3D Printable PCR Polypropylene Vitrimers for a Sustainable Future

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Global plastic pollution impacts the environment, energy, and climate, prompting the development of innovative recycling and upcycling methods to support a circular economy. This study investigates the use of depolymerized polyethylene terephthalate (PET) from waste as a dynamic crosslinker to enhance the properties of functionalized post-consumer recycled polypropylene (PCR PP).

Through glycolysis, waste PET is converted into bis(2-hydroxyethyl) terephthalate (BHET) with high yield. BHET is then utilized to introduce dynamic covalent bonds in maleated PCR PP via transesterification reactions, achieved through an industrially viable melt extrusion process. The resulting crosslinked PCR PP demonstrates vitrimer-like properties, enabling reprocessability, high dimensional stability, and enhanced mechanical strength (14% increase in yield strength compared to PCR PP) and rheological performance.

Characterization confirms the formation of reversible ester linkages, improving material durability and recyclability without significant phase separation. This approach not only provides value to PET waste by converting it into a functional additive but also enhances polyolefin properties, offering a sustainable circular solution for advanced polymer applications with controlled flow properties. Furthermore, a 3D printed product is successfully fabricated using a Fused Granulate Fabrication (FGF) robotic 3D printer, a process not feasible with PCR PP due to its high melt flow index from chain scission during processing.

This work demonstrates the potential of depolymerized polymers as dynamic crosslinkers for creating high-performance, reprocessable materials, promoting both environmental and economic sustainability.

Keywords: Upcycling, PCR PP, Waste PET, 3D Printing.

Low-temperature Fabricated Solution-processed Diodes for Wireless Paper Electronics

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In today's innovative world, where plastic and electronic waste are significantly impacting global climate and human health, a shift towards eco-friendly paper electronics can help reduce the footprint of nonbiodegradable electronic technologies. Herein, we demonstrate an integrated wireless power storage system (IWPSS) that integrates a printed diode and a micro-supercapacitor for paper-based electronic devices. In this system, an inkjet-printed diode on paper wirelessly charges a screen-printed micro-supercapacitor.

To fabricate the diode with an unprecedented high current-carrying capability of 6 A cm^{-2} at 1 V, we developed a method to form a surfactant-free semiconductor film of polycrystalline indium gallium oxide (IGO) nanoparticles at a low thermal budget suitable for the paper substrate. These paper diodes can rectify AC signals up to 10 MHz, with a 3 dB cutoff frequency of 1 MHz. The printed paper diode successfully charges a bulk supercapacitor with an energy density of 8.1 Wh kg^{-1} and a specific capacitance of 28.9 F cm^{-2}, reaching 420 mV in 30 minutes.

Keywords: Inkjet printing, Diodes, Indium Gallium Oxide (IGO), Paper electronics.

Mechanism and Mitigation of Crack Formation in Laser-based Directed Energy Deposition of γ-TiAl Powder

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Lightweight γ-TiAl alloy finds application in advanced aircraft and automobile engines. Though it has attractive properties, it suffers from poor processability through conventional routes like casting and forming. Directed Energy Deposition (DED) is a widely used method for printing and cost-effective remanufacturing of damaged complex parts. However, deposition of γ-TiAl alloy using a laser source is challenging due to rapid cooling caused by convection in an argon atmosphere.

It is observed that Ti4822, a second-generation alloy, undergoes α solidification and forms a fully lamellar or duplex structure depending on process parameters in the as-printed condition. EBSD texture measurement shows the Blackburn orientation relationship between the γ and α_2 phases in the lamellar structure. This study focuses on identifying possible mechanisms responsible for crack formation during the powder-based laser DED process. Systematic investigations have been conducted to examine the influence of process parameters, alloy composition, and microstructure on the crack susceptibility of as-printed parts.

Alloy modification through in-situ alloying with Ti and Al resulted in a crack-free build. Preferential cracking of the γ-phase due to tensile residual stress was observed. Enriching with the α_2-Ti_3Al phase through process parameter control and alloying eliminated crack formation. Processing strategies for achieving crack-free components are proposed based on the findings of this study.

Keywords: Titanium Aluminide, Directed Energy Deposition, Cracking Mechanism, In-situ Alloying.

3D Bioprinted Metastatic Niches of Triple Negative Breast Cancer for Drug Screening

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Triple Negative Breast Cancer (TNBC) is an aggressive breast cancer subtype that often metastasizes to visceral organs such as the lungs, liver, and brain rather than bone. However, the role of the mechanical properties of these secondary sites in TNBC progression and drug resistance is poorly understood, and suitable 3D cell culture models are lacking. This study aims to bridge this gap by utilizing a 3D bioprinted TNBC cell culture model that simulates the biomechanical properties of the extracellular matrix (ECM) found in metastatic sites.

Two Biosteriolithography (DLP)-based bioinks were developed for this purpose: G7.5 and G12.5, with varying gelatin methacryloyl concentrations, exhibiting compressive moduli of 6.7 ±2.5 kPa and 43.8 ±18.4 kPa, respectively. G7.5 mimics the stiffness of lung tissue, while G12.5 reflects high-grade invasive ductal carcinoma and cancellous bone. The TNBC cell line MDA-MB-231 bioprinted in these scaffolds displayed distinct morphologies; cells in G7.5 were more spindle-shaped by day 14 compared to those in G12.5. Metabolic activity increased significantly in G7.5 by day 14 (approximately 3.8-fold), while it remained stable in G12.5 (1.3-fold).

In drug response assays, doxorubicin caused 45% cell death in G7.5 at an IC_{50} of 1 μM, compared to only 20% in G12.5, highlighting the influence of cellular states due to varied mechanical environments on drug efficacy. Overall, the study presents digital light processing (DLP)-based bioinks that effectively replicate ECM mechanical properties affecting the drug response and cellular behavior in TNBC metastatic sites.

Keywords: Breast Cancer, Mechanical Niches, Metastasis, Bioprinting.

Exploring the State-of-the-Art in Quantum Computing for Computational Materials Science

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Quantum computing is emerging as a transformative paradigm in computation, with quantum chemistry and materials science among the leading fields poised to benefit from potential "quantum advantage." However, with the current scale and quality of quantum hardware, the size of the systems that can be practically addressed remains limited. While recent studies have explored applications in molecular systems, research on solids is still scarce.

This work investigates the utility of quantum algorithms in *ab initio* calculations for solids. Furthermore, the accuracy and computational speedup achievable for critical materials science applications, such as surface reactions and adsorption energy calculations, remain largely unexplored. The primary objective of this study is to rigorously analyze and benchmark the accuracy and performance of state-of-the-art quantum algorithms, such as the Variational Quantum Eigensolver (VQE) and quantum-centric supercomputing architectures, against established classical approaches like Density Functional Theory (DFT).

Keywords: Quantum Computing, Variational Quantum Eigensolver, Quantum-centric Supercomputing.

Fabrication and Analysis of Oxide-Based Ferroelectric Gated Transistors Using the Inkjet-Printing Technique

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Printed electronics offer a sustainable alternative to conventional photolithography by significantly minimizing material waste and enabling eco-friendly manufacturing. This approach involves depositing ink on various substrates, including paper, textiles, glass, and polymers, making it ideal for flexible and wearable devices. Among printing techniques, inkjet printing stands out as a digital, additive process that applies material only where needed, reducing waste and eliminating the need for masks or screens. It preserves delicate surfaces and achieves cost reductions of up to 64% compared to traditional methods.

Inkjet printing facilitates the fabrication of uniform, high-performance memristors without photolithography, addressing environmental and efficiency challenges in electronics manufacturing. In this study, solution-based synthesis routes, specifically the inkjet printing technique, were used to fabricate ferroelectric gated transistors (FETs). The successful demonstration of all-printed ferroelectric gate transistors offers a high-throughput, low-cost, low-waste, and sustainable fabrication protocol.

This work successfully demonstrated a single-phase potassium sodium niobate (KNN). The fabricated phase-pure KNN was used to prepare a capacitor structure to optimize its ferroelectric properties. Subsequently, ferroelectric transistors were fabricated and characterized for their electrical performance, including a stable hysteresis window. The aim is to achieve a ferroelectric transistor with substantial electrical properties, such as a memory window, I_{on}/I_{off} ratio, switching speed, and threshold voltage.

Keywords: Ferroelectric transistor, Inkjet printing, Transparent oxide devices, Potassium sodium niobate (KNN).

Simultaneous Increase of d_{33} and Curie Point of PZT by Dilute Rare Earth Doping: The Phenomenon and the Mechanism

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Ever since the discovery of large electromechanical response at the morphotropic phase boundary of the classical piezoceramic system $PbZr_yTi_{1-y}O_3$ (PZT) more than six decades ago, different variants of PZT have been widely used in various applications. For stability of the electromechanical performance of piezoelectric devices against inadvertent temperature increases during operation, the use of piezoceramics with a high Curie point is desirable. In general, chemical modifications of ferroelectrics that significantly improve their piezoelectric response tend to lower the Curie point or depolarization temperature.

Contrary to this general trend, we report a phenomenon wherein slight Eu modification of PZT, synthesized as per the nominal formula $Pb_{1-3x/2}Eu_x(Zr_{0.53}Ti_{0.47})O_3$, not only increases its piezoelectric charge coefficient (d_{33}) remarkably from 204 pC/N (x = 0) to 415 pC/N (x = 0.005), but also raises the Curie point from 373 °C (x = 0) to 389 °C (x = 0.005).

We investigate this phenomenon and its underlying mechanism by analyzing the structures at local and global length scales using a combination of tools such as Eu^{3+} photoluminescence, Raman spectroscopy, and X-ray powder diffraction. We found that the increase in the Curie point is caused by Eu doping, which pushes the system from a two-phase (rhombohedral + tetragonal) state to a single-phase tetragonal state with increased tetragonality. The remarkable increase in d_{33} is associated with Eu enhancing local structural heterogeneity by limiting the field-driven tetragonal → rhombohedral transformation on the local scale. We found the same phenomenon occurring even with dilute doping of PZT using Sm and La.

Keywords: PZT, Electromechanical behavior, Curie point, Crystal structure.

Screen Printed Micro-Supercapacitors on Paper with Additive-Free 1T MoS_2 Ink for Sustainable Energy Solutions

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This study introduces a novel binder-free 1T MoS_2 symmetric micro-supercapacitor (1T-MoS_2 SMSC) fabricated on a flexible paper substrate. By fine-tuning the geometry of the electrode fingers and employing a quasi-solid 3M PVA-H_2SO_4 electrolyte, we have achieved high capacitance and excellent cyclic stability across various operational conditions.

Electrochemical characterization, including cyclic voltammetry (CV) and chronopotentiometry (CP), revealed that the 1T-MoS_2 SMSC maintains nearly quasi-rectangular CV curves, indicating an ideal capacitive behavior. The device demonstrated a high areal capacitance of 5.5 mF cm^{-2} at 2 mV s^{-1}. In addition, series connections of the devices have shown promising performance metrics suitable for portable electronic applications, achieving significant energy and power density values.

Keywords: 1T MoS_2, Areal capacitance, Binder-free electrode, Flexible micro-supercapacitor.

Influence of Transition Metal Doping on the Exciton Dynamics in All-Inorganic Metal Halide Perovskite

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All-inorganic metal halide perovskites ($CsPbX_3$) have been extensively studied due to their exceptional optical and photovoltaic characteristics, rendering them promising candidates for next-generation optoelectronic applications. Transition metal (TM) ion doping has been identified as a viable approach to enhance material performance and broaden their practical utilization. However, a detailed quantitative understanding of the influence of transition metal ions on the band structure, defect states, exciton dynamics, and the overall modulation of optical properties is yet to be fully realized.

In this work, the hot-injection method was employed to synthesize pure $CsPbX_3$ and transition metal-doped $CsPb_{(1-y)}TM_yX_3$ nanocrystals (NCs). XRD studies revealed an orthorhombic phase of the NCs and increased strain in the doped sample. Luminescence in these materials is primarily dictated by free exciton (FE) recombination, though additional emission peaks were consistently observed. By systematically optimizing growth temperature and doping concentrations, we achieved tunable luminescence while preserving the intrinsic bandgap structure.

Room-temperature photoluminescence (PL) and time-resolved PL (TRPL) analyses revealed an extended charge carrier decay lifetime in doped samples compared to pristine $CsPbX_3$. Additionally, at cryogenic temperatures ($T < 130K$), a broad emission peak emerged at the lower energy tail, coexisting with the free excitonic peak. This phenomenon is ascribed to self-trapped excitons (STEs) and phonon-assisted scattering processes. These insights contribute to a deeper comprehension of charge carrier interactions and doping strategies in $CsPbX_3$ perovskite nanocrystals, potentially informing future material design and application development.

Keywords: All-inorganic metal halide perovskite, Transition metal ions, Self-trapped excitons, Temperature-dependent photoluminescence.

Diffusion Analysis in Binary and Ternary Ni-Based Alloys Following Experimental, Density Functional Theory (DFT), and Physics-Informed Neural Network Numerical Inverse Method (PINN)

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Most of the experimental diffusion studies available in the literature are in binary systems. Diffusion studies in ternary systems have been very limited until now. Moreover, the interdiffusion coefficients are calculated mainly in ternary systems. However, these diffusion parameters are a kind of average of intrinsic diffusion coefficients of elements and may not correctly reflect the actual diffusional interactions between the elements.

In this study, we have extensively studied binary Ni-X and ternary Ni-Al-X (X=Cr, Mo, W, Ta, Re) systems, estimating tracer, intrinsic, and interdiffusion coefficients at different temperatures. The data in ternary systems are estimated following the conventional method by intersecting diffusion paths and a recently established method of direct estimation at the Kirkendall marker plane from a single diffusion profile. Estimation following different methods for generating similar data confirms the reliability of mobility data produced in this study.

Further, the comparison of diffusion coefficients between binary and ternary systems indicates a very useful understanding of the role of Al, which is an integral part of Ni-based superalloys. These experimental studies are complemented with density functional theory (DFT) analysis, highlighting the atomic mechanism of diffusion by discussing the dominating role of atomic size or electronic configuration. Finally, a physics-informed neural network numerical (PINN) method is utilized for the generation of composition and temperature-dependent mobility databases in correlation to the experimentally estimated diffusion coefficients.

Keywords: Diffusion, DFT, PINN.

Proton Irradiation Effects on Multi-Principal Element Alloy

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This study explores the irradiation behavior of a low stacking fault energy (SFE) variant of the Cantor alloy (equiatomic CoCrFeMnNi), a multi-principal element alloy (MPEA). Proton irradiation was performed at room temperature (RT) with a 6.5 MeV beam energy at a dose of 5×10^{17} p/cm^2. SRIM (Stopping and Range of Ions in Matter) simulations for this irradiation condition indicated a peak damage level of approximately 0.16 dpa, located around 135 μm from the irradiated surface.

Nanoindentation tests revealed irradiation-induced hardening, with hardness increasing from an unirradiated baseline of 2.76 $\pm$0.1 GPa to 3.66 $\pm$0.1 GPa at 50 μm depth and 4.47 $\pm$0.1 GPa at 135 μm depth in the irradiated cross-section. Transmission electron microscopy (TEM) analysis at 30-50 μm and 120-135 μm depths showed irradiation-induced dislocation loops, with a higher loop density at 120-135 μm, explaining the observed depth-dependent hardening.

Post-irradiation deformation investigations beneath nano-indent impressions revealed dislocation pinning and bowing at these loops. Hardness estimates using the dispersion barrier hardening (DBH) model aligned well with the experimental measurements. Post-irradiation annealing (PIA) at 200 °C for 6 and 24 hours showed no significant effect on hardness, while annealing at 400, 500, and 550 °C for 0.5 hours demonstrated a clear trend of hardness recovery.

Keywords: Multi-principal element alloys, Proton irradiation, Dislocation loops, Nanoindentation.

Development of High Strength and High Conductivity Cu-Ag Based Alloys

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The development of copper alloys that combine both high strength and high conductivity presents a significant challenge in materials science, driven by the growing demand for efficient electrical components in advanced technologies. Achieving a favorable balance between strength and conductivity typically involves modifying the microstructure through solid solution, precipitation, dispersion, and deformation strengthening. Among these methods, precipitation strengthening is one of the most effective approaches.

In this study, a Cu-Ag-Cr-Ge alloy has been developed using rapid solidification processing followed by various heat treatments to enhance both strength and conductivity. A notable finding is that the addition of chromium and germanium causes the microstructure to transition from discontinuous (seen in the Cu-Ag binary alloy) to continuous precipitation, leading to a 54% increase in tensile strength. This improvement is attributed to solid solution strengthening from aluminum in the matrix, as well as the formation of Ag-rich and Cr-rich precipitates.

The precipitate's crystal structure and composition were further analyzed using scanning/transmission electron microscopy (SEM/TEM) and atom probe tomography (APT) for a deeper understanding.

Keywords: Cu-alloys, Strength, Electrical conductivity, SEM, TEM, APT.

Towards Single Crystal Growth in CMSX-4 Superalloy Builds Using Laser Directed Energy Deposition

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Single crystalline Ni-based superalloys are preferred in the hottest parts of aero-engines due to the absence of grain boundaries, which improves high-temperature creep strength. Conventionally, directional solidification (DS) processing is used to produce columnar and single crystalline (SX) microstructures in Ni-based superalloys. However, traditional manufacturing involves multiple complicated steps and requires long-term homogenization heat treatments before the component can be used in its final application.

Additive manufacturing (AM) has revolutionized the manufacturing sector due to its ability to produce near-net-shaped components in a single step using a computer-aided design (CAD) model. In addition, the high thermal gradients and solidification rates associated with AM processing favor epitaxial growth and result in microstructural refinement compared to conventional processing. The objective of this study is to identify the parameter space that promotes epitaxial growth in CMSX-4 superalloy builds using the Laser-based Directed Energy Deposition (L-DED) additive manufacturing process. A FormAlloy L-DED machine is used to fabricate CMSX-4 superalloy single crystals with [001] orientation by epitaxial growth from the substrate. A bi-directional scan strategy is employed, with key parameters such as laser power, scanning speed, powder flow rate, and layer height systematically varied. Microstructural and crystallographic analyses are conducted to understand the solidification behavior in relation to L-DED process parameters. In-depth analysis reveals that dynamic adjustments to process parameters are crucial for initiating and sustaining epitaxial growth while preserving the build's topology.

Keywords: Single crystal, Laser-based additive manufacturing, Epitaxial growth, CMSX-4.

A DFT Study of Hydrogen Interstitial Solute Interaction with Dislocations in Nickel

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Ni-based alloys are used extensively in aerospace, nuclear, oil and gas, and chemical processing industries. Several Ni-based alloys, including IN718, A286, and IN625, have shown potential to replace relatively low-strength austenitic stainless steels in high-pressure hydrogen environments, particularly for applications requiring strength at high temperatures. Hydrogen segregation to dislocations and the associated changes in dislocation mobility are closely related to embrittlement. In this study, segregation of atomic hydrogen to dislocations and stacking faults was analyzed using density functional theory (DFT) (VASP v. 5.2 within the MEDEA framework).

To this effect, we estimated the binding energy of hydrogen atoms at different sites in the vicinity of dislocations and stacking faults. The binding energy was calculated for the strain field (from the anisotropic elastic theory of dislocations) corresponding to a perfect straight edge dislocation, a straight extended edge dislocation, a perfect straight screw dislocation, and an extended screw dislocation. These binding energy calculations explicitly account for the volumetric and shear distortions due to hydrogen in octahedral and tetrahedral sites in an elastically anisotropic material.

A machine learning algorithm was further used to predict the binding energy around the dislocations and determine the equilibrium composition in these regions. The results were compared against classical theory predictions, which involve isotropic strain fields while considering volumetric distortions. The study revealed significant deviations from classical theory, emphasizing the importance of accounting for elastic anisotropy and shear distortions in hydrogen-dislocation interactions.

Keywords: Hydrogen embrittlement, Dislocation interactions, Density functional theory, Elastic anisotropy.

Impact of Ge as an Alloying Addition on Microstructure and High-Temperature Mechanical Properties of 2nd Generation TiAl Alloy

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This work studies the effect of Ge addition on the microstructure and high-temperature mechanical properties of Ti-48Al-2Cr-2Nb alloys. It is shown that Ge improves mechanical properties through precipitate strengthening and solid solution strengthening, though the contribution of solid solution strengthening was not significant.

Four alloys were examined in this study: Ti-48Al-2Cr-2Nb (at.%), Ti-48Al-2Cr-2Nb-0.5Ge (at.%), Ti-48Al-2Cr-2Nb-0.75Ge (at.%), and Ti-48Al-2Cr-2Nb-1Ge (at.%). The first two alloys showed similar microstructures after homogenization. However, upon adding 0.75 at.% and 1 at.% Ge, precipitates started forming at colony boundaries and lamellar interfaces. The precipitate volume fraction increased with higher Ge concentrations.

High-temperature compressive and creep properties of Ti-48Al-2Cr-2Nb and Ti-48Al-2Cr-2Nb-0.5Ge (at.%) were almost identical, indicating a minimal solid solution effect of Ge. Excellent compressive and creep properties were observed in the Ti-48Al-2Cr-2Nb-0.75Ge (at.%) alloy. TEM studies revealed significant twin activity in the 0.75Ge-containing TiAl alloy compared to the base alloy. Creep-deformed microstructure analysis showed dislocation pile-up near the precipitates, which led to a decreased steady-state creep rate in the 2nd-generation TiAl alloy.

Keywords: Precipitate strengthening, Twinning, Creep.

Development of Tunable Ferroelectric Thin Films for Bandpass Filters in Satellite Systems

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This project aims to develop ferroelectric-based thin films that function as high, low, and band-pass filters within the microwave frequency range, with potential applications in satellite systems. The dielectric permittivity (ε) of dielectric/ferroelectric materials is strongly dependent on the applied bias electric field. This characteristic property, known as tunability, is crucial for a variety of applications. Ferroelectrics are distinguished by their high dielectric constant and tunability. In this study, we have grown a thin film of composition $0.25BiFeO_3$-$0.30BaTiO_3$-$0.45SrTiO_3$ (BFBST) on an Nb:STO (001) substrate using Pulsed Laser Deposition (PLD) and fabricated a coplanar waveguide (CPW) architecture via photolithography. We performed microwave radio frequency (RF) characterization (500 MHz to 10 GHz) of this device using a vector network analyzer (VNA). A one-port measurement (reflection coefficient S_{11}) was conducted to calculate the dielectric constant of BFBST.

Upon applying an external bias, variations in the dielectric constant were observed, reaching a tunability of 72% at 2 GHz under 200 V. The tangent loss (< 1) was calculated for varying voltage levels, demonstrating low dielectric loss, which is favorable for RF applications. Hafnia-based ferroelectrics, particularly doped hafnium oxide (HfO_2), have garnered significant attention due to their compatibility with complementary metal-oxide-semiconductor (CMOS) technology. These materials exhibit robust ferroelectric properties at nanoscale (10 nm) dimensions.

Our future objective is to integrate Zr-doped HfO_2 (HZO) with BFBST to develop a microwave tunable filter.

Keywords: Ferroelectric thin films, Microwave tunability, CMOS compatibility, Space satellite applications, Band-pass filters.

Wafer-Scale Solution-Processed 2D-TMD Transistors and Circuits Enabled by Single-Flake Transport

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Wafer-scale uniform deposition of 2D materials has emerged as a critical focus for both vacuum and solution-based processing due to the broad applications in large-area electronics. However, solution-processed 2D electronics have been constrained by challenges such as device-to-device variability and performance limitations. These solution-processed 2D thin-film transistors (TFTs) and circuits often suffer from low charge carrier mobility due to junction resistance between randomly assembled small flakes, which impedes carrier transport. Traditional solution-processing methods, such as printing, slot-die coating, and Langmuir-Blodgett assembly, rely only on fluidic mechanics to deposit uniform layers of 2D materials. However, these methods struggle to achieve precise single-flake assembly within the active regions of TFTs.

Here, we present a novel fabrication approach for large-area, solution-processed 2D transistors that enables single-flake transport by leveraging non-uniform electric fields to attract individual flakes of 2D materials to the channel region. This method allows the assembly of high-quality 2D materials with low post-processing temperatures (<120 °C), making it compatible with a wide range of flexible substrates and expanding its potential applications in flexible and wearable electronics. The technique's ability to minimize junction resistance between flakes enhances carrier mobility and addresses a critical bottleneck in solution-processed 2D electronics.

To assess their reliability for practical applications, the devices underwent extensive stability tests, including evaluations of bias stability, cyclic stability, switching stability, environmental stability, and strain tolerance. Furthermore, this electric field-assisted assembly has been successfully extended to fabricate logic gates and digital circuits, highlighting its scalability and reliability.

Keywords: Large-area electronics, Junction resistance, 2D electronics, Dielectrophoresis.

Engineering 3D Bio-Printed Lung-on-a-Dish Platform to Investigate Pulmonary Fibrosis

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Idiopathic Pulmonary Fibrosis (IPF) is an interstitial lung disease that results in excessive deposition of collagen in the lung alveoli regions. The lack of understanding of several key aspects of cell interactions has prevented us from obtaining a better treatment option. Processes underlying this unusual disease remain poorly understood due to the absence of dependable and reproducible models reiterating tissue pathophysiology. The underlying limitations of such models underscore the development of a clinically relevant 3D *in vitro* model. It will be used to understand the associated biological pathways, determine key molecular players, and later be used as an accurate drug screening platform.

3D bio-printing has emerged as the latest frontier in tissue engineering and regenerative medicine. A GelMA, alginate, and methylcellulose-based bioink was optimized and characterized for physicochemical and mechanical properties. This was followed by 3D bioprinting parameter optimization at different cell densities and cross-linking times. The cell viability, proliferation, and morphological features in a 3D culture were compared over two weeks.

Our approach aims to create a biomimetic microsystem that reconstitutes the functional alveolar interface of the human lung. It will help us understand the epithelial-to-mesenchymal transition of epithelial cells and the stimulation of fibroblasts as they progress toward the myofibroblast stage. In the future, we will introduce multiple *in vivo* parameters, such as cyclic breathing patterns and fluid flow in the system, to better resemble human lungs.

Keywords: 3D model, Lung alveoli, Fibrosis, A549.

Nature of Morphotropic Phase Boundary in the Lead-Free Piezoelectric Systems $K_{1/2}Bi_{1/2}(M_{1/3}Nb_{2/3})_xTi_{1-x}O_3$: M = Mg, Zn

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The lead-free piezoelectric system $(K_{1/2}Bi_{1/2})(Mg_{1/3}Nb_{2/3})O_3$ -$(K_{1/2}Bi_{1/2})TiO_3$ (KBMN-KBT) has recently been reported to show a composition-driven tetragonal (P4mm)-monoclinic (Pm) inter-ferroelectric instability, similar to what is known for the Pb-based piezoelectric system $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN-PT). This has led to the view that KBMN-KBT is a Pb-free analogue of PMN-PT. We critically examine this view by analyzing the structural states of compositions near the proposed morphotropic phase boundary of KBMN-KBT. To ensure generality, we also investigate the Zn-analogue $(K_{1/2}Bi_{1/2})(Zn_{1/3}Nb_{2/3})O_3$-$(K_{1/2}Bi_{1/2})TiO_3$ (KBZN-KBT) system.

In conjunction with dielectric, ferroelectric, and piezoelectric measurements, we performed structural analysis at different length scales using X-ray diffraction, Raman spectroscopy, and transmission electron microscopy techniques. We identified two distinct critical compositions: one corresponding to the maximum weak-field piezoelectric response (d_{33}) and another corresponding to the maximum large-field converse piezoelectric coefficient (d^*_{33}). Unlike PMN/PZN-PT, the maximum electromechanical response in KBMN/KBZN-KBT is not associated with a symmetry-breaking structural-polar instability. Instead, the increased electromechanical response is caused by the onset of a microstructural (domain) instability leading to the formation of short-range order (SRO) ferroelectric domains of the same tetragonal (P4mm) symmetry.

We establish a correlation between the electrostrain response and the electric-field-driven reversible short-range to long-range order transformation. Our study provides key insights into the important differences between KBMN/KBZN-KBT and their proposed Pb-based counterparts, both from structural and property viewpoints.

Keywords: Piezoelectricity, Structure-property correlation, Lead-free piezoceramics.

Room Temperature Creep in Ti6242

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Dwell fatigue in titanium alloys at room temperature is significantly influenced by room temperature (RT) creep, which occurs despite titanium's high melting temperature. This study investigates the mechanisms governing RT creep through interrupted creep tests, where specimens were subjected to controlled loading followed by detailed microstructural analysis.
Scanning electron microscopy (SEM) was employed to capture deformation characteristics, while slip trace analysis using Electron Backscatter Diffraction (EBSD) provided insights into the active slip systems. By correlating observed slip traces with crystallographic orientations, the study identifies dominant deformation mechanisms contributing to RT creep and time-independent deformation. Microstructural features influencing creep behavior, such as grain orientation and slip transmission across boundaries, were examined. Understanding these mechanisms provides crucial insights into the underlying processes that drive RT creep in titanium alloys.
These results have implications for the fatigue performance of titanium components, particularly in applications where dwell loading is critical. By advancing knowledge of RT creep behavior, this study contributes to the development of improved alloy design for dwell fatigue-resistant Ti alloys.

Keywords: Titanium alloys, Room temperature creep, Dwell fatigue, SEM, EBSD.

Harnessing Excited-State Charge Transfer for the Activation of Dark Triplet Excitons and Phosphorescence in Hybrid Organic-Inorganic 2D Perovskite

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In recent years, room temperature phosphorescence (RTP) materials have been the subject of intense research, driven by their potential uses in diverse areas, including optoelectronics, time-gated bio-imaging, anticounterfeiting, and sensing applications. We introduced a novel hybrid organic-inorganic 2D perovskite, where a rational molecular design strategy enables efficient triplet exciton generation through an excited-state charge transfer (ESCT) process.

Upon photoexcitation, a sharp and intense emission peak with a narrow bandwidth is observed at $\sim$ 400 nm, reflecting excitonic emission from the perovskite entity, which subsequently undergoes charge transfer to the energetically aligned triplet state of the organic spacer molecule. The triplet state (T_1) of the spacer molecule then undergoes radiative intersystem crossing (ISC) to the ground state (S_0), resulting in efficient broad phosphorescence emission at $\sim$ 560 nm, with an excited state lifetime of $\sim$ 30 milliseconds under ambient atmosphere, suggesting excellent moisture stability of the 2D perovskite.

Furthermore, the overlap of the phosphorescence spectra of the organic spacer molecule and the 2D perovskite provides additional evidence supporting our proposed excited-state charge transfer mechanism. Collectively, the temperature-dependent steady-state photoluminescence, photoluminescence excitation (PLE) spectra, and delayed luminescence studies provide strong evidence for our proposed mechanistic framework of understanding the excited-state dynamics in hybrid organic-inorganic 2D perovskite.

Keywords: Intersystem crossing, Phosphorescence, 2D perovskites, ESCT.

Enhancing Fatigue Resistance of Cr-Mn-Fe-Co-Ni System by Varying Composition and Sigma-Phase Assisted Grain-Size Reduction

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This study investigates two key aspects of the low cycle fatigue (LCF) behavior of alloys from the Cr-Mn-Fe-Co-Ni system at room temperature: (1) the influence of stacking fault energy (SFE) in single-phase face-centered cubic (FCC) alloys and (2) a grain size reduction triggered by the precipitation of a small amount of σ-phase.

The first effect is studied using model alloys ($Cr_{26}Mn_{20}Fe_{20}Co_{20}Ni_{14}$ and $Cr_{14}Mn_{20}Fe_{20}Co_{20}Ni_{26}$ in at.%, grain size: $\sim$60 µm), which exhibit distinct SFEs at room temperature. A reduction in SFE from 69 to 23 mJ/m^2 results in a 10 – 20% increase in tensile/compressive peak stresses, i.e., cyclic strength, across all examined strain amplitudes ($\pm$0.3%, $\pm$0.5%, and $\pm$0.7%) while maintaining comparable fatigue lives. Despite its higher cyclic strength, the low-SFE alloy exhibits delayed and less evolved dislocation substructures compared to the other alloy.

By aging the $Cr_{26}Mn_{20}Fe_{20}Co_{20}Ni_{14}$ alloy differently, we induced the precipitation of $\sim$5% σ-phase during recrystallization, which significantly reduced the FCC grain size to $\sim$5 µm. With this refined microstructure, cyclic strength increased by 50 – 65% and remained more stable during fatigue testing while maintaining a comparable fatigue life. The σ-precipitates effectively deflected and arrested fatigue cracks, while extensive deformation twinning around cracks complemented slip activity and reduced the crack propagation rate.

Overall, σ-phase-assisted grain size reduction is 3 – 5 times more effective in improving cyclic strength than SFE reduction.

Keywords: Multi-principal element alloys (MPEAs), Stacking fault energy, Low-cycle fatigue (LCF), Deformation and damage mechanisms.

Simultaneous Enhancement of d_{33} and Depolarization Temperature of the Morphotropic Phase Boundary Composition of the Pb-Free Piezoceramic $Na_{1/2}Bi_{1/2}TiO_3$ – $BaTiO_3$

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We investigate the influence of the oxygen-deficient modifier $BaAlO_{2.5}$ (BAO) on the structure, dielectric, and piezoelectric properties of the morphotropic phase boundary (MPB) composition $Na_{1/2}Bi_{1/2}TiO_3$-6.5$BaTiO_3$ (NBT-6.5BT) in the lead-free NBT-BT piezoceramic solid solution. The weak signal longitudinal piezoelectric coefficient (d_{33}) and the depolarization temperature (T_d) of the MPB NBT-6.5BT piezoceramic are approximately 150 pC/N and 90 °C, respectively. In general, chemical modification strategies that enhance d_{33} in NBT-BT tend to reduce the depolarization temperature. Contrary to this trend, we demonstrate that it is possible to improve both d_{33} and T_d of NBT-6.5BT ceramics. We found that merely 1 mole percent of BAO increases the d_{33} to 205 pC/N, accompanied by a remarkable increase in the T_d to 160 °C.

Keywords: Pb-free piezoceramic, Depolarization temperature, Morphotropic phase boundary.

Semi-Solid TIG-Based Additive Manufacturing of Al-15Mg_2Si-4.5Si-0.01Sr-0.015B Composite

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Semi-solid Tungsten Inert Gas (TIG)-based Additive Manufacturing (AM) presents a promising approach for fabricating high-performance aluminum matrix composites with refined microstructures and enhanced mechanical properties. In this study, the feasibility of processing an Al-15Mg_2Si-4.5Si-0.01Sr-0.015B composite using semi-solid TIG-AM is explored.

The composite composition is tailored to achieve a uniform distribution of Mg_2Si particles and refined eutectic Si, with Sr and B acting as modifiers and grain refiners, respectively. By leveraging the semi-solid state during deposition, the process mitigates common defects associated with conventional AM techniques, such as hot cracking and excessive porosity, while promoting controlled solidification and microstructural homogeneity.

Detailed analyses of the microstructure, phase evolution, and mechanical properties are conducted to assess the effectiveness of the approach. The findings demonstrate that semi-solid TIG-AM enables the fabrication of Al-15Mg_2Si-based composites with improved hardness, strength, and ductility, making it a viable technique for advanced structural applications.

Keywords: Semi-solid processing, TIG-based additive manufacturing, Al-Mg_2Si composites, Grain refinement.

Effect of Reduction Per Pass During High-Temperature Rolling of Mg-1wt%Gd Alloy on Texture, Mechanical, and Corrosion Properties

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The effect of rolling reduction per pass on the texture, mechanical, and corrosion properties of Mg-1wt%Gd alloy was investigated in this study. Mg alloyed with Gd exhibits the highest solid solubility among rare earth-based alloys, leading to notable texture modifications.

Three different processing routes were employed to generate distinct textures through high-temperature deformation. The as-cast alloy was homogenized and subjected to rolling under three different conditions:

- Route 1: 20% per pass reduction,
- Route 2: 50% per pass reduction,
- Route 3: Variable per pass reduction.

For the rolling stage, the alloy was heated to 470ÂřC for 30 minutes before rolling from 12 mm to 1.2 mm thickness (90% reduction). The microstructural and textural evolution of the processed materials was examined on the ND-RD plane using optical microscopy, SEM, EBSD mapping, and on the ND-TD plane via XRD pole figures.

Microstructural analysis revealed that Route 3 led to enhanced grain refinement and a weaker basal texture compared to Route 1 and Route 2. A strong correlation was established between microstructure, texture evolution, mechanical behavior, and corrosion resistance.

Keywords: Mg alloy deformation, Mg rare earth textures, Mechanical behavior, Microstructure-texture correlation, Hot rolling, Rare earth alloying, Corrosion of Mg rare-earth alloys.

A Roadmap for Producing Single-Crystal Ni-Based Superalloy Components Using Laser-Directed Energy Deposition Process

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Additive manufacturing (AM) has emerged as a transformative approach for fabricating geometrically complex components, particularly in aerospace applications. High-pressure turbine blades in jet engines present a unique challenge, requiring both intricate designs and stringent single-crystallinity to ensure optimal performance. Achieving these specifications through AM demands precise control over process parameters to promote single-crystal growth while maintaining structural integrity.

In this study, we present a multi-scale modeling and experimental framework to identify the optimal parameters for single-crystalline builds using Laser-Directed Energy Deposition (L-DED). At the process scale, a diffuse-interface-inspired model predicts melt pool dynamics and thermal histories during multi-layer deposition. These thermal conditions serve as inputs for a Potts-based microstructure model to analyze grain evolution and solidification texture. By coupling process simulations with grain-scale modeling, we delineate a parameter space conducive to epitaxial single-crystal growth.

Experimental validation confirms that the identified process conditions yield single-crystalline structures. Additionally, phase-field simulations incorporating full CMSX-4 alloy composition predict primary dendrite arm spacing (PDAS), which aligns with experimental measurements, reinforcing the accuracy of our solidification model. This integrated computational-experimental approach enhances our understanding of process-microstructure relationships, providing a pathway for optimizing additive manufacturing strategies for complex single-crystal components.

Keywords: Additive manufacturing, L-DED, Single-crystal Ni superalloy, Modelling and simulation.

Experimentally Validated and Empirically Compared Machine Learning Approach for Predicting Yield Strength of Additively Manufactured Multi-Principal Element Alloys

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Traditionally, yield strength prediction relies on detailed and resource-intensive microstructural characterization combined with empirical equations. However, quantifying microstructural feature length scales for novel processes like additive manufacturing (AM), which involves inhomogeneous hierarchical features, poses a significant challenge. The lack of accurate material constants for broader composition ranges further limits empirical predictions.

This study proposes an alternative machine learning (ML) approach for predicting the yield strength of additively manufactured multi-principal element alloys (MPEAs) from the Co-Cr-Fe-Mn-Ni system by correlating composition, printing parameters, and testing conditions. The top-performing ML model achieved an R^2 value of 0.84, comparable to the best microstructure-based empirical strengthening model.

The ambiguities and inconsistencies associated with empirical methods in the literature were critically evaluated for the $Co_{33.3}Cr_{33.3}Ni_{33.3}$ alloy. The validity of the ML approach was further confirmed by printing and testing two compositions (one novel and one from the dataset). This data-driven approach directly relates yield strength to initial printing parameters, highlighting their significance and individual effects, such as scan velocity's direct impact and laser power's inverse impact on yield strength.

This study demonstrates ML's potential to guide AM processes, reducing the need for iterative experiments and enabling rapid exploration of compositional and printing spaces to achieve desired properties.

Keywords: Additive manufacturing, Multi-principal element alloys, Yield strength, Machine learning.

Upcycling Post-Consumer Recyclate of Polyamide 66 by Controlling Chain Scission and Crosslinking Density

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According to contemporary estimates, over 400 Mt of plastic is created annually, with polymer waste accounting for 70%. This contributes significantly to plastic pollution. Statistics suggest that approximately 16% of all plastic waste is recycled. There remains a substantial amount of mismanaged polymer waste and its resulting carbon footprint. A closed-loop circular economy in polymers is necessary to address polymer mismanagement and ensure sustainability.

This work effectively discloses the upcycling of Post-Consumer Recyclate (PCR) nylon Polyamide 66 (PA66), obtained from automotive regrind and fishing nets, which were not previously addressed from a closed-loop perspective. To the best of our knowledge, this is the first study to report dynamically crosslinked polyamides with enhanced strength and reprocessability.

In the presence of a Lewis acid, multi-functional amines crosslink polyamide via transamidation and end-group condensation, thereby imparting functional properties to PCR PA66. The mechanical performance of the resulting crosslinked system was tested, and the maximum was attained at a loading rate of 5 wt%, which is almost 28% higher than neat PCR samples. The mechanical properties did not degrade even after three reprocessing cycles.

The prepared system exhibited fast stress relaxation, lasting 20.67 seconds at 260 °C and 5.88 seconds at 290 °C. The thermal stability of the developed systems was not affected by crosslinker loading. This work opens new opportunities for recycling PA66 and will guide the research community toward new material and process protocols.

Keywords: Polyamide 66, Post-consumer recycling, Crosslinked polyamides, Circular economy.

Poster Abstracts

Edge States in Quasi-2D Halide Perovskites: Sites of Efficient Exciton Dissociation

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In the realm of perovskite optoelectronics, understanding how excitons behave at crystal edges is key to unlocking high-performance photovoltaics. Quasi-two-dimensional (2D) layered halide perovskites harbor the unique property of enhanced exciton dissociation at crystal edges, known as localized edge states. These crystal edges, along with grain boundaries and free surfaces, serve as sites where excitons – bound pairs of electrons and holes – dissociate into free carriers, enhanced by thermal disorder and dangling octahedral bonds present at these locations.

Photogenerated excitons from the bulk diffuse to these localized edge states, where they dissociate into longer-lived free carriers, improving conductivity at these sites. This high population of free carriers is then extracted by the respective transport layer and collected at the electrodes, improving power conversion efficiency. By carefully controlling the population of edge states at the interface between the perovskite and transport layer, we can significantly boost the power conversion efficiency of quasi-2D layered halide perovskites, bringing us closer to more stable, high-performance photovoltaic devices.

As Nobel Laureate Herbert Kroemer famously said, "The Interface is the Device." This holds true in the realm of perovskite optoelectronics, where interface behavior can make all the difference in device performance.

Keywords: Quasi-2D perovskites, Exciton dissociation, Edge states, Photovoltaics.

A Numerical Analysis of Solidification Microstructure Dependence on Solidification Characteristics in Laser-Based Additive Manufacturing

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The dependence of alloy microstructure on cooling rates is well known in the literature. However, with the advent of additive manufacturing, where components are built layer by layer using a heat source such as a laser, electron beam, or arc to melt metal powders or wires, very high cooling/solidification rates can be achieved. The evolution of microstructures under such processing conditions is not well understood.

This work aims to compare and understand the evolution of microstructures in single-track melt pools under varying processing parameters during Laser Powder Bed Fusion (LPBF) for three industrially important alloys: Inconel 718, AlSi10Mg, and 316L stainless steel. The differences in alloy thermodynamics, kinetics, and thermal solidification characteristics such as thermal gradients and cooling rates are responsible for variations in grain morphologies, texture evolution, size distributions, and defects.

This study highlights the differences observed in additively manufactured single-track experiments across these alloy systems, emphasizing their impact on mechanical performance.

Keywords: Microstructure, Additive manufacturing, Laser powder bed fusion, Single tracks.

Accelerated High Entropy Alloy Design for Corrosion Resistance Using First Principles Calculations and Data-Driven Techniques

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High Entropy Alloys (HEAs) of the Fe-Ni-Cr-Co-Mn system are being investigated as cost-effective substitutes for Ni-based alloys (e.g., Hastelloy-N) with superior corrosion resistance and mechanical performance in molten salt environments. Unlike conventional alloys, which typically have one or two base elements, HEAs consist of five or more elements in nearly equal proportions, leading to unique structural and property variations.

In this study, Face-Centered Cubic (FCC) Special Quasi-Random Structures (SQS) were generated for a range of disordered binary, ternary, and quaternary alloy compositions using the Sqsgen package. These structures were analyzed using Density Functional Theory (DFT)-based first-principles calculations to determine equilibrium lattice parameters, bulk modulus, cohesive energy, and surface properties such as surface energies for (100), (110), and (111) crystallographic planes. The generated data was utilized to develop machine learning models for predicting key material properties, including bulk modulus, surface energy, and cohesive energy across binary, ternary, and quaternary compositional ranges. Advanced regression models, such as Random Forest and Gradient Boosting, were employed to enhance prediction accuracy, with hyperparameter optimization and cross-validation ensuring model robustness. The entire compositional space was explored using high-throughput techniques, with ternary plots visualizing property trends. Furthermore, a Genetic Algorithm-based multi-objective optimization framework was developed to identify compositions with high resistance to molten salt corrosion while maintaining desirable mechanical properties for applications in nuclear reactors.

Keywords: High Entropy Alloy, SQS Structures, First-Principles Calculation, Machine Learning Models.

3D Printing of Medical-Grade Silicone Elastomer for Personalized Soft Tissue Implants

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Prostheses and implants constitute essential components within contemporary healthcare frameworks. Silicones, also called silicone rubber, have been widely employed in medical device production due to their chemical inertness, tissue-like mechanical properties, and adaptability. However, structural complexity and specificity constraints limit conventional routes for processing silicones. The emergence of three-dimensional (3D) printing technologies for silicones has become a crucial avenue for creating patient-specific and intricately engineered implants and prostheses.

Despite ongoing research in 3D printing of silicones, the employment of medical-grade silicones, which are predominant in the biomedical domain, presents multiple challenges. This work focuses on the 3D printing of medical-grade silicones utilizing a customized printer, wherein various parameters were systematically modified to evaluate the printability of silicones and the printed parts' physicochemical properties. The print bed temperature and layer orientation were varied to analyze their effects on mechanical properties, leachable or extractable substances, defect or void formation, and cytotoxicity of the 3D-printed silicones.

The mechanical assessment of the specimens revealed that a print bed temperature of 90 °C, with a print orientation of 45°, yielded the lowest values for tensile strength and modulus. X-ray micro-computed tomography (µCT) analysis corroborated these results by characterizing porosity and quantifying the pore volume fraction. Nuclear Magnetic Resonance (NMR) studies revealed that some precursors were leaching out, but these did not induce cytotoxicity. Together, these results demonstrate the viability of 3D printing of medical-grade silicones for biomedical applications.

Keywords: Silicone, Additive manufacturing, Mechanical properties, Biomaterials.

Improving Fatigue Resistance of a Bainitic Steel by Exploiting Segregation-Induced Bands

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An ultrafine bainitic steel was designed with segregation-induced martensitic/austenitic (MA) bands. The steel comprises almost 21% retained austenite (RA), with the rest mainly consisting of bainitic ferrite and a small fraction of martensite. The steel exhibits a room temperature (RT) yield strength of ∼914 MPa, an ultimate tensile strength of ∼1969 MPa, and a total elongation to failure of ∼11.5%.

Low-cycle fatigue (LCF) behavior was investigated under a fully reversed strain-controlled waveform at RT, with the loading axis parallel to the MA bands. The LCF stress response reveals initial cyclic hardening followed by softening or saturation, depending on the applied strain amplitude. This is attributed to the interplay of strengthening mechanisms, including RA transforming to martensite and dislocation multiplication/interactions, counterbalanced by the softening effects of dislocation annihilation and crack formation/propagation.

Damage studies reveal a mixed fracture mode, displaying brittle striations, secondary cracks, quasi-cleavage facets, and dimples. The secondary cracks primarily originate from the main crack and propagate predominantly along the matrix-bands interphase regions or within MA bands. Additionally, surface-initiated cracks along their propagation path were deflected and branched around the interphase regions. This tortuosity reduces the crack propagation rate.

Overall, the significant work hardening capability of the steel, along with its banded microstructure, contributes to its superior fatigue resistance compared to non-banded bainitic steels reported in the literature.

Keywords: Bainite, Martensite/austenite (MA), Low-cycle fatigue (LCF), Cracks.

Estimation and Characterization of Fatigue Threshold

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Estimation and characterization of the fatigue threshold are essential for predicting and designing various components used in engineering applications. Several testing methods are available in the literature to estimate the fatigue threshold, but the main limitation of these methods is the mixing of intrinsic fatigue threshold with crack closure, known as the extrinsic fatigue threshold. In this investigation, a new method has been applied to naval steel for estimating the intrinsic fatigue threshold ($\Delta K_{th,i}$) in the absence of crack closure.

The intrinsic fatigue threshold has been estimated as a function of near-tip residual stress (σ^*), which can be controlled by periodic overloads. The relationship between the intrinsic fatigue threshold and near-tip residual stress exhibits a good correlation at a particular distance (r^*) from the crack tip. Additional tests with higher overloads have been conducted, revealing that crack closure could play a significant role, and its effect must be considered for accurate estimation of the intrinsic fatigue threshold ($\Delta K_{th,i}$).

Furthermore, the fractographic study indicates curved crack fronts due to higher overloads and larger plastic zones. The crack extension during periodic overload cycles is minimal (0.25 micron). This research contributes to the accurate estimation of both intrinsic and extrinsic fatigue thresholds, which can help improve the prediction capabilities of existing fatigue crack propagation models.

Keywords: Fatigue threshold, Crack closure, Near-tip residual stress, Variable amplitude loading.

Determination of Elastic Stiffness Constants using Nanoindentation

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The nanoindentation technique has been widely used for determining hardness and elastic modulus. These material properties are typically obtained using the Oliver and Pharr methodology. However, the conventional equations for modulus extraction are only valid for isotropic materials. For anisotropic materials, a modified approach by Vlassak and Nix introduces indentation modulus (M), which is a function of elastic stiffness constants (C_{ijkl}) and the orientation of the indented surface (hkl).

For polycrystalline materials where the grain size is much smaller than the indent size, the conventional approach remains valid. However, when the grain size is larger than the indent size, indentation is effectively performed on a single crystal at a particular orientation, necessitating the use of the modified equation.

This work addresses the inverse problem of determining elastic stiffness constants from nanoindentation data. Since the relationship between indentation modulus, stiffness constants, and crystallographic orientation is complex, optimization methods implemented through MATLAB were employed to solve this problem. The methodology was tested on materials with face-centered cubic (FCC) and hexagonal close-packed (HCP) crystal structures, such as copper and titanium. The results showed that the approach works well for cubic systems. However, in hexagonal systems, where the number of independent stiffness constants is higher, obtaining a unique solution for the optimization problem remains challenging.

Keywords: Nanoindentation, Elastic stiffness constants, Anisotropy.

Role of Gadolinium Addition on Slip Activity and Slip Transfer in Pure Magnesium

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This study investigates the role of the rare-earth element Gadolinium (Gd) addition on the anisotropic mechanical response and deformation mechanisms in pure magnesium. The investigated alloy, Mg-1.5Gd, was extruded at 400 °C followed by annealing to obtain a recrystallized microstructure with a similar grain size (75 Âţm). Incorporating 1.5 wt.% Gd in pure Mg leads to a pronounced reduction in basal texture. Consequently, Gd addition increases ductility up to 50%, while eliminating the tension-compression yield asymmetry.

Furthermore, to elucidate the active deformation mechanisms, a statistical investigation of the operating slip modes over a large area containing 500 grains was carried out under tension using EBSD-assisted slip trace analysis. The interrupted tensile specimens of Mg-Gd at two different strains reveal a 55% increase in non-basal slip activity with increasing strain from 3% to 8%. Apart from slip activity, the similar twinned area fraction of 21.3% under both tension and compression indicates the activation of similar deformation mechanisms in the Mg-Gd alloy.

The slip transfer/blocking analysis also showed that slip transfer is likely to occur if the Luster-Morris factor (m) > 0.7. In contrast, cases where slip transfer is difficult (m < 0.7) are more prone to cracking at grain boundaries.

Keywords: Deformation mechanism, Tension-compression asymmetry, Slip trace analysis, Slip transfer analysis.

Phase Distribution in Quasi-2D Dion-Jacobson Perovskite Dictates Ultrafast Charge Build-up and Directional Charge Transfer

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The efficient and rapid charge transfer at the interface of heterostructures plays a crucial role in optoelectronic applications. Quasi-2D perovskites, featuring randomly dispersed phases of varying layer thickness (n), introduce multiple interfaces with potential barriers that hinder charge transfer. This study demonstrates a strategic spatial distribution of various n-phases, enhancing charge transfer while enabling narrow-band emission in high-n phases.

It was found that the additive CsI alters the phase distribution across the films. Notably, strong radiative emissions from low-n phases were observed at low temperatures, despite their absence at room temperature. The phenomenon of ultrafast charge transfer and charge build-up in consecutive phases was observed in quasi-2D perovskite thin films. Photocurrent reduction in these films further confirmed the anisotropic nature of charge transfer. Additionally, the reduction in local surface potential upon illumination corroborates the role of spatial phase distribution in promoting directional charge transfer.

Keywords: Quasi-2D, Directional Charge Transport, Charge Funneling.

Computational Modeling of Stacking Fault Energy in Nickel and Nickel-based Alloys

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Face-centered cubic (FCC) metals exhibit partial dislocations due to low-energy planar defects like stacking faults, which influence dislocation behavior and deformation mechanisms. This work focuses on computational modeling of stacking fault energies in metals and alloys, particularly in technologically significant Ni-based superalloys used in turbine engines for their superior high-temperature strength and corrosion resistance. Given the complexity of modeling multi-component superalloys, we begin with pure Ni and extend to binary Ni-Co alloys.

We employ first-principles-based density functional theory (DFT) as our computational methodology. We apply two different approaches to model intrinsic stacking faults: (1) the direct supercell approach, and (2) the alias shear deformation approach. While the direct supercell approach allows us to calculate only the intrinsic stacking fault energies, the alias shear deformation approach can estimate so-called generalized stacking fault energy (GSFE) curves, a theoretical concept describing the energy dependence of shearing a (111) plane of an FCC crystal along a [1ÌĚ12] slip direction. To model Ni-Co alloys, we explore the Special Quasi-random Structure (SQS) approach to generate alloy structures emulating disordered solid solutions within the supercell approach with periodic boundary conditions.

We estimate similar (difference within 2%) intrinsic stacking fault energies (γ_{ISFE}) in Ni using both the direct supercell and alias shear deformation approaches. Our estimated value of γ_{ISFE}, 123.8 mJ/m^2, compares very well with experiments (120 - 130 mJ/m^2), as well as with previous DFT literature (127.2 - 133.0 mJ/m^2). We find that having the correct magnetic ground state of Ni in stacking fault energy calculations is important for quantitative comparison with experiments.

Keywords: Ni-based alloys, Stacking fault energies, Density Functional Theory, One-dimensional axial Ising Model.

Morphology-Dependent Luminescence Property of $CsPbBr_3$ 3D Perovskite

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$CsPbX_3$ perovskite semiconductors have been extensively studied over the last decade due to their excellent optical properties and applications in various fields. In this study, photoluminescence (PL) emission properties, defect states, and recombination mechanisms in different morphologies of $CsPbBr_3$ were investigated using steady-state and time-resolved PL spectroscopy in the temperature range of 80K to 300K.

It was found that the exciton binding energy obtained from PL intensity depends on quantum confinement and varies with dimensionality. Additionally, the PL lifetime increases with increasing temperature. Temperature-dependent time-resolved PL (TRPL) measurements further enhance the understanding of exciton trapping and de-trapping processes in nanocrystals with various morphologies.

Keywords: $CsPbBr_3$, Perovskite, Photoluminescence, Quantum confinement, TRPL.

The Heat Treatment of Additively Manufactured Ti-35Nb-7Zr-5Ta Alloy for Orthopedic Applications

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The increasing demand for orthopedic implants has driven research into advanced biomaterials with superior mechanical properties, biocompatibility, and corrosion resistance. This study focuses on the heat treatment of an additively manufactured Ti-35Nb-7Zr-5Ta alloy fabricated using the Directed Energy Deposition (DED) process to enhance its structural and mechanical performance.

The as-printed samples were characterized for their microstructure, phase composition, and mechanical properties. Subsequent heat treatments were conducted at 900ÂřC and 1000ÂřC for varying durations, followed by water quenching, to achieve chemical homogeneity and optimize the microstructure. Electron microscopy, X-ray diffraction (XRD), and micro-hardness testing were employed to analyze the effects of heat treatment.

The study confirmed that heat treatment at 1000ÂřC significantly improved elemental homogeneity and retained the β-phase, leading to an increase in hardness. Further aging at 480ÂřC resulted in precipitation hardening, enhancing mechanical strength. Additionally, surface mechanical attrition treatment (SMAT) induced nanocrystallization, further improving hardness due to increased dislocation density.

The findings suggest that controlled heat treatment and surface modifications can effectively optimize the mechanical properties of Ti-35Nb-7Zr-5Ta alloys for biomedical applications. This research provides valuable insights into the processing-structure-property relationships in additively manufactured titanium alloys, paving the way for their improved performance in orthopedic applications.

Keywords: DED, SMAT, XRD, Ti-35Nb-7Zr-5Ta Alloy.

Carbon Nanoparticles for Cancer Theragnosis

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Cancer remains one of the leading causes of mortality worldwide. Continuous advancements in treatment strategies are needed to improve patient outcomes. Current therapies include chemotherapy, brachytherapy, immunotherapy, and phototherapy. However, chemotherapy is often associated with limitations such as off-target effects and multi-drug resistance.

Phototherapy is emerging as a promising treatment modality and encompasses photodynamic and photothermal therapy. Photodynamic therapy utilizes photoactive materials that, upon activation by radiation, exhibit therapeutic effects. In contrast, photothermal therapy employs a radiation source to generate heat for tumor ablation.

We synthesized carbon nanoparticles using a green chemistry approach, which, when administered via intra-tumoral injection, are activated upon exposure to near-infrared light. This activation leads to the emission of phonons, causing localized heat generation and selective tumor ablation. As cancer cells are more prone to apoptosis due to heat generation, this process results in selective cancer cell death while sparing healthy cells.

The localized surface plasmon resonance effect is responsible for the generation of heat, involving the excitation of valence-shell electrons of the atom upon exposure to specific wavelengths of light. Additionally, the fluorescence property of the nanoparticles was employed for real-time monitoring of tumor mass, highlighting their “theranostic ”potential.

The synthesized nanoparticles were characterized for their size, morphology, surface charge, functional groups, elemental composition, and photo-activable properties. These nanoparticles possess the potential to serve as a synergistic treatment modality for cancer, alongside existing therapeutic options.

Keywords: Cancer, Phototherapy, Carbon nanoparticle, Theragnosis.

Effect of Temperature on Dwell Fatigue in Near Alpha Ti-6242 Alloy

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Ti-6Al-2Sn-4Zr-2Mo is a near-alpha titanium alloy used in turbine engine blades and disks, where operational conditions involve high stresses around 800 – 900 MPa and temperatures of 120âĹŠ200ÂřC. These alloys are susceptible to dwell fatigue, which significantly shortens their service life.

The objective of this study is to investigate how temperature influences the dwell fatigue behavior of Ti-6242 within the specified temperature range. Additionally, an associated creep study is conducted at each temperature level, as creep plays a crucial role in the dwell effect during fatigue cycles. Low-cycle fatigue (LCF) tests are performed to analyze and compare LCF and dwell fatigue (DF) at similar temperatures.

An unusual temperature effect is observed in both creep and fatigue behavior. Anelastic recovery during unloading is seen at 200 °C in low-cycle fatigue testing, a phenomenon absent at room temperature. This behavior is further examined through loading-unloading tests and back-stress measurements.

The dwell fatigue results indicate reduced strain accumulation at 200 °C, which is analyzed in conjunction with creep results obtained at both room temperature and 200 °C. To further understand these unusual temperature effects on creep, stress relaxation, strain rate jump, and stress jump experiments are conducted at both temperatures. The stress relaxation results align with the creep observations. Strain rate sensitivity does not exhibit notable variations with temperature. The activation volumes measured at these temperatures suggest a shift in deformation mechanisms.

Keywords: Titanium alloy, Dwell fatigue, Low-cycle fatigue, Creep.

Tribological Behaviour of Surface Mechanical Attrition Treatment-Based Mg-Zn Alloys for Biomedical Applications

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Magnesium (Mg) alloys, particularly Mg-Zn (0.4 and 2 wt.% Zn), have garnered considerable attention for biomedical applications due to their favorable biodegradability and biocompatibility. However, their inherent low wear resistance and mechanical strength remain significant challenges in load-bearing applications.

This study investigates enhancing the tribological behavior of Mg-Zn alloys through Surface Mechanical Attrition Treatment (SMAT). SMAT, a surface modification technique, was employed to refine the surface microstructure and improve hardness. Under conditions simulating the physiological environment, the treated and untreated alloys were subjected to comprehensive tribological tests, including sliding wear against alumina balls. Wear rates, friction coefficients, and surface roughness were analyzed, with results indicating a marked improvement in wear resistance and friction behavior of SMAT-treated Mg-Zn alloys compared to untreated samples. Microstructural analysis via scanning electron microscopy (SEM) and X-ray diffraction (XRD) confirmed grain refinement and the formation of a hardened surface layer post-treatment. The enhanced tribological performance is attributed to the increased hardness and refined microstructure, which mitigates wear mechanisms in Mg alloys. These findings suggest that SMAT-treated Mg-Zn alloys offer promising potential for biomedical implants, particularly in orthopedic applications where improved wear resistance is crucial.

Keywords: Wear, SMAT, Mg-Zn alloys, Orthopedic applications.

Development of Machine Learning Interatomic Potentials for High-Performance Cathode Materials in Magnesium Batteries

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Magnesium batteries offer several distinct advantages over traditional lithium-ion batteries, including superior volumetric energy density, enhanced safety profiles, and lower cost due to the abundant natural availability of magnesium. However, a major challenge in advancing magnesium battery technology lies in the development of high-performance cathode materials that can facilitate efficient Mg^{2+} insertion.

In this study, we employed Moment Tensor Potentials (MTPs) to accurately capture the interatomic interactions within Mg-based cathode materials. The training dataset for MTP was generated using *ab initio* molecular dynamics (AIMD) simulations, modeling the amorphous phases of MgV_2O_5 and V_2O_5. The MTP parameters were optimized to replicate density functional theory (DFT)-calculated energies and forces, achieving training root-mean-square errors of 0.004 eV/atom for energy and 0.24 eV/Åfor force.

The trained potential was subsequently validated against the DFT database and applied in large-scale molecular dynamics simulations to compute Mg-ion diffusivity. The results demonstrate the capability of the developed computational framework to predict material behavior accurately across different atomic configurations and thermal conditions, highlighting the potential of MTPs as a powerful tool for designing high-performance cathode materials for magnesium batteries.

Keywords: Magnesium Batteries, Moment Tensor Potentials (MTPs), Molecular Dynamics.

Diffusion Study in Ni-Based System Using Experimental and a Physics-Informed Machine Learning-Based Numerical Inverse Method

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Ni-Al-based alloys are extensively used in high-temperature applications such as gas turbines and jet engines due to their superior mechanical properties and resistance to corrosion and oxidation. Diffusion studies are crucial as they control key physical and mechanical properties that ultimately limit the life of these materials. A critical aspect influencing these properties is diffusion, particularly its role in precipitate formation and mechanical degradation over time. Most diffusion studies have been concentrated on binary systems, with limited investigations in ternary systems.

In this study, we estimate diffusion coefficients in the Ni-Co-Cr-Al-Ti system for the first time. Initially, diffusion analyses were performed in binary and ternary systems before extending the study to multicomponent systems. Additionally, the Hall method was utilized to estimate impurity diffusion coefficients. Experimentally, diffusion coefficients can only be determined at specific compositions (i.e., at the intersections of diffusion paths and the Kirkendall marker plane).

To overcome this limitation, a physics-informed neural network (PINN) model was developed to optimize and extract diffusion coefficients across the entire composition range of diffusion couples. Experimentally estimated diffusion coefficients at specific compositions were used as constraints to improve the reliability of the extracted data, preventing numerical methods from generating random values. The data generated in this study is further extended to correlate with coarsening kinetics that govern creep and degradation in Ni-based alloys.

Keywords: Diffusion, Ni-Al-based alloy, PINN.

Exploring Cryogenic and Room-Temperature Performance of Additively Manufactured CoCrNi Alloys: Influence of Stacking Fault Energy

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Multi-principal element alloys (MPEAs), particularly the CoCrNi system, possess outstanding mechanical properties, including an excellent strength-ductility balance, making them ideal for cryogenic applications. The composition and associated stacking fault energies (SFEs) significantly influence the deformation mechanisms, thereby affecting the overall mechanical performance. This study examines the tensile behavior of additively manufactured non-equiatomic Co-Cr-Ni alloys, emphasizing the role of SFE on their mechanical properties and deformation mechanisms at both room temperature and cryogenic conditions (77K).

At room temperature, the high SFE alloy deformed primarily through slip, whereas the low SFE alloy exhibited both slip and twinning, leading to an enhanced strength-ductility combination. Under cryogenic conditions, twinning also supported slip in the high SFE alloy. In contrast, the low SFE alloy exhibited a combination of slip, twinning-induced plasticity (TWIP), and transformation-induced plasticity (TRIP). Notably, the high SFE composition achieved exceptional ductility of 74% at 77K, whereas the low SFE composition demonstrated an impressive tensile strength of 1 GPa.

This study underscores the potential of optimizing tensile properties in the CoCrNi system by tailoring SFE through compositional modifications. The findings provide valuable guidelines for developing advanced materials for aerospace and energy applications.

Keywords: Multi-principal element alloys (MPEAs), TWIP, TRIP, Tensile property.

Impact of Surface Mechanical Attrition Treatment on Microstructural and Mechanical Properties of WAAM-Manufactured AISI 304

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Additive manufacturing (AM) has gained significant importance in the production of metallic structural elements for various engineering applications. While research has primarily focused on powder-based processes, there is still limited knowledge concerning the structural response and mechanical properties of wire-and-arc additive manufactured (WAAM) metallic components.

This study investigates the influence of surface mechanical attrition treatment (SMAT) on the microstructural and mechanical properties of WAAM-fabricated AISI 304 stainless steel. Five different depositions were produced under varying conditions, and porosity testing using Archimedes' principle was performed to evaluate densification. Among the samples, the deposition at 170A exhibited the highest densification.

Microstructural characterization via X-ray diffraction (XRD) revealed the presence of ferrite and austenite phases, while optical microscopy provided detailed insights into dendritic grain structures aligned along the building direction. SMAT was subsequently applied to the WAAM-printed SS304 samples to enhance their mechanical properties.

Post-SMAT characterization demonstrated significant changes in phase composition and stress distribution. XRD analysis revealed the formation of deformation-induced phases and the generation of compressive stresses, as evidenced by the rightward peak shifts of austenite and ferrite phases. This comprehensive evaluation highlights the potential of SMAT in improving the performance of WAAM-fabricated SS304, paving the way for applications requiring superior mechanical properties.

Keywords: WAAM, SMAT, XRD, SS304.

Understanding the Polaron Dynamics in 2D Ruddlesden-Popper Perovskite

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The efficiency of two-dimensional Ruddlesden-Popper-type materials relies on the complex interplay between electronic and lattice dynamics; however, questions remain about how growth conditions manipulate exciton – phonon interactions. Here, we establish the different polaronic nature of the excitons in these growth-modified materials by combining ultrafast transient absorption spectroscopy, low-frequency resonance Raman spectroscopy, and time-domain terahertz spectroscopy.

We show that polaronic distortion is associated with low-frequency (1-2 THz) lead iodide octahedral lattice motions. More importantly, we discover how the growth conditions of this two-dimensional perovskite structure manipulate exciton – phonon coupling, exciton polaron population, and carrier cooling. The annealed material shows longer-lived polarons compared to the as-grown material.

Our study provides detailed insight into the effect of growth conditions on exciton – phonon coupling and its role in carrier cooling in two-dimensional perovskites, which is relevant for developing emerging hybrid semiconductor materials with tailored properties.

Keywords: 2D Perovskite, Exciton-Phonon Coupling, Polaron Dynamics, Spectroscopy.

Bio-waste to Bio-ink for 3D Bio-printing: Treatment of Tympanic Membrane Perforation to Restore Hearing Loss

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The Tympanic Membrane (TM) serves as the interface between the middle and external ear, converting sound waves into mechanical vibrations to facilitate hearing. The function of the TM depends on its unique structure, composition, and mechanobiology. Structural disruptions due to perforation or rupture – caused by microbial infections, ventilation tube extrusion, significant accidents, explosions, trauma, or congenital disabilities – can result in acute to chronic hearing disorders and even conductive hearing loss.

The severity of TM perforations (TMPs) is classified into four grades (Grade I-IV). While Grades I-II TMPs are acute and typically heal within weeks with medical attention, Grades III-IV TMPs often fail to regenerate naturally, leading to severe chronic conditions requiring surgical intervention such as tympanoplasty. Over the years, xenografts and autologous tissues have been used in grafting procedures to restore hearing. However, these approaches present disadvantages such as mechanobiological mismatches, surgical trauma, postoperative complications, potential rejection, and high costs. Additionally, patients often experience persistent hearing impairment despite intervention.

To address these limitations, this research explores a tissue engineering-based solution leveraging 3D bioprinting techniques and bio-waste. Specifically, placenta-extracted bio-ink is utilized to fabricate a 3D bio-printed, customized bio-adhesive patch. This patch functions as a localized extracellular matrix (ECM), stimulating progenitor and local cells to accelerate natural healing without the need for invasive surgeries or expensive treatments.

Keywords: Bio-waste, Bio-ink, 3D-Printing, Tympanic Membrane Perforations (TMPs).

Molecular Docking of Antibiotics with Target Enzymes for the Design of Effective Antibiotic Sensors

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Molecular docking studies play a significant role in understanding the interactions between antibiotics and enzymes, which are pivotal in developing sensors for effective therapeutic strategies. This study focuses on docking antibiotics with their target enzymes in humans to predict the binding affinities responsible for their interactions.

From the docking results, we observed specific amino acids that interact with the antibiotics, providing insights into the binding affinity and specificity. These observations are instrumental in deriving molecules that can simulate the enzymatic affinity for its interactions with antibiotics. The design and development of such molecules hold significant promise for enhancing the sensing of antibiotics and overcoming the risks posed by antibiotic resistance.

This work emphasizes the importance of molecular docking in sensor development. It underscores the potential to advance the understanding of antibiotic-enzyme interactions, thereby aiding in the design and development of sensors for the selective sensing of antibiotics used for specific bacterial strains to combat global bacterial resistance.

Keywords: Molecular docking, Antibiotic, Enzyme.

Effect of Ytterbium Addition and Surface Modification on the Corrosion and Mechanical Properties of Mg-Zn-Ca Alloy for Biomedical Applications

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Magnesium alloys have gained significant attention as potential biomedical implant materials for orthopedic applications due to their biocompatibility, biodegradability, and mechanical properties comparable to human bone. However, the high corrosion rate of Mg limits its application in biomedical devices. Alloying elements can mitigate the corrosion rate of Mg by forming secondary phases that hinder corrosion.

Calcium (Ca) and Zinc (Zn) are preferred alloying elements due to their biological compatibility and role in various physiological functions. Additionally, rare earth (RE) elements have been reported to improve the corrosion resistance of Mg alloys. This study investigates the effect of ytterbium (Yb) on the microstructure, mechanical properties, and corrosion behavior of the Mg-1.5Zn-0.5Ca-xYb system, where Yb content is varied at 0.75%, 2%, and 5%. The alloy containing 2% Yb exhibited the best combination of properties and was selected for further characterization and surface modification.

Surface modification significantly influences the mechanical properties and corrosion behavior of metallic implants. This study employs the Surface Mechanical Attrition Treatment (SMAT), a severe plastic deformation (S2PD) process, to enhance the performance of the Mg-1.5Zn-0.5Ca-2Yb alloy. The study aims to understand the effect of SMAT on mechanical strengthening and corrosion resistance, making Mg alloys more viable for biomedical implant applications in orthopedic surgery.

Keywords: Magnesium alloy, Ytterbium, Surface Mechanical Attrition Treatment (SMAT), Corrosion, Biomedical implants.

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