RESEARCH
SCHOLARS' DAY

ABSTRACT
BOOKLET

Department of
Materials Science and Engineering
IIT Kanpur

pdaर्थ

Department of
Materials Science and Engineering

IIT Kanpur

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About the Department

Established in 1960, the Department of Materials Science and Engineering at IIT Kanpur is recognized as one of the leading centers for education and research in materials science and engineering in the country. The department was originally founded as the Department of Metallurgical Engineering and launched its postgraduate program in 1964. Over the decades, the department has continuously evolved to meet the changing needs of society and advancements in technology. Reflecting this evolution, it was renamed Materials and Metallurgical Engineering in 1993, and later transitioned to the Department of Materials Science and Engineering in 2009.

Since its inception, the department has remained committed to nurturing young minds and promoting intellectual growth through high-quality education and research. This commitment is reflected in its strong emphasis on fundamental principles, supported by an interdisciplinary curriculum that integrates various aspects of materials science and engineering. The department is known for its cutting-edge research across diverse areas of materials science, supported by a distinguished faculty and well-structured academic programs.

Today, the department offers a highly regarded undergraduate program and a vibrant graduate program, attracting talented students from across the country and beyond. Its alumni network spans both national and international institutions, comprising accomplished professionals and researchers who continue to contribute significantly to academia, industry, and technological innovation.

Message from the Head of the Department

Welcome to Research Scholars' Day (RSD) 2026, organised by the Department of Materials Science and Engineering (MSE), IIT Kanpur, on March 14-15, 2026. RSD is a humble initiative aimed at providing a platform for the research scholars of the MSE department to present their impactful outcomes, challenging initiatives, and discuss innovative ideas of their research journey at IIT Kanpur. Such student-driven academic activities help create a stimulating environment where scholars can exchange novel thoughts, learn from peers, and strengthen research culture in the department.

The enthusiasm in preparation and the energy of participation are clearly visible and have inspired everyone involved. With the registration of 45+ student participants from across the department, a plenary talk by distinguished expert ***Prof. Siddhartha Misra***, Tata Steel, and keynote talks by ***Prof. Sanjay Mittal***, IIT Kanpur, and ***Prof. Vivek Verma***, IIT Kanpur will undeniably spark curiosity and encourage reflection on the way we understand our world. In addition, ***Prof. Anoop Krishnan***, IIT Delhi, is organising a workshop on *AI/ML in Materials Science* that has set the tone for the event.

The *eight* technical sessions of RSD 2026 highlight the diverse research activities carried out within the department, covering a broad spectrum of materials science and engineering. These themes include emerging areas such as modelling and simulation in materials science and engineering, functional and energy materials and biomaterials and bioengineering, along with *core areas of metallurgy*, *materials processing*, *extractive metallurgy and corrosion of metals, and physical and mechanical behaviour of materials*. Together, these themes reflect the department's interdisciplinary approach towards advancing both fundamental understanding and technological applications of materials. Two parallel sessions on both days demonstrate the strong technical focus of RSD 2026. I am confident that this event will provide an excellent platform for research scholars to showcase their work, exchange ideas, and foster meaningful academic discussions within the department.

I extend a sincere note of gratitude to all the student members for their leadership, unparalleled support from faculty colleagues and strong assistance from staff members. We also extend our sincere thanks to our sponsors, Macro Systems, RR Enterprises, Virtual Labs, Global Computers and local vendors who have come forward to support the cause. The support from affiliated department technical societies, i.e. Material Advantage at IIT Kanpur, Indian Institute of Metals Kanpur Chapter, and Materials Science Society, is also appreciated.

Roots have deepened, and the sense of ownership has grown stronger. RSD has become a cherished tradition of the Department of Materials Science and Engineering, IIT Kanpur.

We look forward to welcoming you to experience RSD 2026 with us!

Best wishes
Prof. Kantesh Balani

MESSAGE

Message from Organizers, RSD 2026, IIT Kanpur

Prof. Rahul Sarkar
Convenor
(RSD 2026)

Prof. Heena Khanchandani
Convenor
(RSD 2026)

Prof. Srinu Gangolu
Treasurer
(RSD 2026)

Prof. Arunabh Meshram
Secretory

Prof. Niraj Chawake
Advisor

The Research Scholars' Day (RSD) is envisioned as an event by research scholars for research scholars a platform dedicated to fostering academic exchange, collaboration, and innovation in metallurgy and materials science. Building on the success of previous editions, we are pleased to present RSD-2026, hosted by the Department of Materials Science and Engineering, Indian Institute of Technology Kanpur, on March 14-15, 2026.

Continuing on its mission, RSD-2026 provides young researchers with an opportunity to showcase their latest research, engage in meaningful discussions, and strengthen collaborations within the research community. The event will feature plenary and keynote lectures by distinguished members from industry and acdemia, along with oral and poster presentation sessions where research scholars can present their research and exchange ideas with their peers.

In addition, the colloqium will include a hands-on worhsopn on "Artificial Intellegence for End-to-End Materials Modelling and Discovery ". Finally, we hope, it will act as a platform to encourage discussions amongst the scholars of the department and to share their perspectives on research challenges, academic growth, and the impact of materials science in modern technological advancements.

We sincerely thank the Department of Materials Science and Engineering, IIT Kanpur, for their continued support in organizing this event. Our heartfelt appreciation goes to the faculty members, staff, and the organizing committee whose dedication and efforts have been instrumental in shaping RSD-2026.

A special note of thanks goes to the dedicated student secrataries and volunteers , the backbone of RSD whose enthusiasm and hard work continue to make this event possible.

Organizing Committee,
RSD-2026

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Technical Sessions-III A(L18): Biomaterials and Bioengineering

Technical Sessions-III B(L18): Modelling and Simulation in Materials Science and Engineering

Poster Presentation(L18 foyer)

Technical Schedule (at glance)
14th March 2026: DAY 1

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<tr><th>Time</th><th colspan="2">Event</th></tr>
<tr><td>9:0-10:00</td><td colspan="2">Registration
(Venue: Infront of L18)</td></tr>
<tr><td>10:00-10:30</td><td colspan="2">Inaugural and Director's Address
(Venue: L18)</td></tr>
<tr><td>10:30-11:15</td><td colspan="2">Plenary Lecture: "Decarbonising the steel industry-one molecule at a time" by Dr. Siddhartha Misra, Tata Steel
(Venue: L18)</td></tr>
<tr><td>11:15-11:50</td><td colspan="2">High Tea
(Venue: Infront of L18)</td></tr>
<tr><td>13:00-14:15</td><td colspan="2">Lunch
(Venue: Infront of L18)</td></tr>
<tr><td rowspan="2">14:30-16:00</td><td colspan="2">Parallel Technical Sessions</td></tr>
<tr><td>Oral Session- I A:
Physical and Mechanical Behaviour of Materials
(Venue: L18)</td><td>Oral Session- I B:
Extractive Metallurgy and Corrosion of Materials
(Venue: L15)</td></tr>
<tr><td>16:00-17:00</td><td colspan="2">3-Minutes Thesis Competition
(Venue: L18)</td></tr>
<tr><td>17:15-19:30</td><td colspan="2">Workshop on "AI/ML in Materials Science" by Prof. Anoop Krishnan, IIT Delhi
(Venue: DJ 204H)</td></tr>
<tr><td>19:45 Onwards</td><td colspan="2">Colloquium Dinner
(Gala dinner for all registered participants and guests)
(Venue: VH1)</td></tr>
</table>

MATERIAL ADVANTAGE IIT KANPUR
IIM Metallurgy Materials Engineering
MATSOC The Materials Society

15th March 2026: DAY 2

<table>
<tr><th>Time</th><th colspan="2">Event</th></tr>
<tr><td>9:30-10:20</td><td colspan="2">Keynote Lecture: "Sustainable Space Exploration: Air Intakes of Reusable Launch Vehicles" by Prof. Sanjay Mittal, IIT Kanpur
(Venue: L18)</td></tr>
<tr><td>10:20-10:45</td><td colspan="2">Tea Break
(Venue: Infront of L18)</td></tr>
<tr><td rowspan="2">10:45-12:45</td><td colspan="2">Parallel Technical Sessions</td></tr>
<tr><td>Oral Session- II A:
Functional and Energy Materials
(Venue: L18)</td><td>Oral Session- II B:
Materials Processing
(Venue: L15)</td></tr>
<tr><td>12:45-14:00</td><td colspan="2">Lunch
(Venue: Infront of L18)</td></tr>
<tr><td>14:15-15:00</td><td colspan="2">Keynote Lecture: "Agar and Cellulose based Dressings for Faster Blood Clotting" by Prof. Vivek Verma, IIT Kanpur
(Venue: L18)</td></tr>
<tr><td rowspan="2">15:00-16:00</td><td colspan="2">Parallel Technical Sessions</td></tr>
<tr><td>Oral Session- III A:
Biomaterials and Bioengineering
(Venue: L18)</td><td>Oral Session- III B:
Modelling and Simulation in Materials Science and Engineering
(Venue: L15)</td></tr>
<tr><td>16:15-17:15</td><td colspan="2">Poster Session and Metallography Contest
(Venue: L18 Foyer)</td></tr>
<tr><td>17:40-18:00</td><td colspan="2">Valedictory & Prize Distribution Ceremony
(Venue: L18)</td></tr>
<tr><td>18:00 Onwards</td><td colspan="2">High Tea</td></tr>
</table>

Time	Event
16:15-17:15	Poster Session and Metallography Contest (Venue: L18 Foyer)
17:40-18:00	Valedictory & Prize Distribution Ceremony (Venue: L18)
18:00 Onwards	High Tea

----------------------------------- End of Day- 2 -----------------------------------

Detailed Oral Presentations Schedule

Day:1	Date: 14th March 2026		Slot: Afternoon (14:30 -15:45)	Venue: L18
Technical Sessions-I A: Physical and Mechanical Behavior of Materials			Title of Presentation	
Session Chairs: Prof. Nilesh Prakash Gurao Prof. Shashank Shekhar				
S.NO	**TIME**	**SPEAKER**		
1	14:30-15:00	Md Irfan Ali	Role of Zn addition on microstructural evolution and mechanical properties of a novel Mg-1.2Al-0.4Ca-0.2Ce alloy processed by rotary swaging	
2	15:00-15:15	Abhishek Kumar	Interface-Controlled Creep in a Non-Equiatomic CoCrNi Alloy with Hierarchical Microstructure.	
3	15:15-15:30	Digbijaya Pradhan	Connectivity-Based Grain Boundary Engineering of FeCoCrNiMn High Entropy Alloy: Effect of Deformation and Annealing on CSL Network Evolution and Corrosion Behavior	
4	15:30-15:45	Sachin Kumar	Investigating Interdiffusion in B2 (Ni, Ru) Al Alloy	
5	15:30-15:45	Kunwar Pratap Singh Yadav	Microstructure and Mechanical Property Correlation in High-Entropy Dual-Phase (Ti,Zr,Ta,Hf) Boride-Carbide-Based Ultra High Temperature Ceramic	

Day:1	Date: 14th March 2026		Slot: Afternoon (14:30 -15:45)	Venue: L15
Technical Sessions-I B: Extractive Metallurgy and Corrosion of Metals			Title of Presentation	
Session Chair: Prof. A.K. Singh				
S.NO	**TIME**	**SPEAKER**		
1	14:30-15:00	Debanjan Gain	Enrichment of Lean-grade Iron Ores using Reduction Roasting for Sustainable Ironmaking	
2	15:00-15:15	Devendra Nama	Reduction behaviour of hematite concentrates under H2 environment in a flash ironmaking reactor	
3	15:15-15:30	Ankur Srivastava	Hydrogen Production through Recycling of Black Aluminium Dross via Alkaline Leaching	
4	15:30-15:45	K Sesha Sai Varma	Effect of pseudomonas aeruginosa on corrosion behavior of mild steel in marine environment	
5	15:45-16:00	Shirish Chandrakar	In-situ investigation on hydrogen-induced deformation micromechanisms in commercially pure titanium	

Research Scholars' Day on Metallurgy and Materials RSD - 2026

Detailed Oral Presentations Schedule

Day:2	Date: 15th March 2026		Slot: Forenoon (10:45 -12:30)	Venue: L18
Technical Sessions-II A:		Functional and Energy Materials	Title of Presentation	
Session Chair: Prof. Sarang Ingole				
S.NO	TIME	SPEAKER		
1	10:45-11:00	Sandipan Bhattachrya	Cold sintering–assisted microstructural engineering of Na3.2+xZr2-xMgxSi2.2P0.8O12 solid electrolytes enabling enhanced Na-metal battery performance	
2	11:00-11:15	Tushar B. Deshmukh	Hierarchically Engraved $NiFePO_4$ Microrods on MWCNTs for Next-Generation Scalable Supercapacitor Electrodes	
3	11:15-11:30	Darshilkumar Chhatrodiya	Investigating partial oxidation of CH4 in CO2-rich environments using Gd0.1Ce0.9O2-δ–SrFe0.9Ti0.1O3-δ composite oxygen transport membranes	
4	11:30-11:45	Aditya Uday Kamat	Tunable insulator–metal transition in epitaxial VO2 thin films via strain and defect engineering	
5	11:45-12:00	Thutta Mohan	Synergistic Enhancement of Lithium-Sulfur Battery Performance via a Sugarcane Bagasse Derived Porous Carbon Sulfur Cathode and a Bi2Se3 Catalytic Interlayer	
6	12:00-12:15	Shiven Ponnapureddy	Sintering Kinetics of Nano Al_2O_3 - 3 mol% Y_2O_3-stabilized ZrO_2 Composites during Intermediate and Final Stages via Spark Plasma Sintering	

Day:2	Date: 15th March 2026		Slot: Forenoon (10:45 -12:30)	Venue: L15
Technical Sessions-II B:		Materials Processing	Title of Presentation	
Session Chair: Prof. Arunabh Meshram				
S.NO	TIME	SPEAKER		
1	10:45-11:00	Shahid Nabi	Liquid Phase Sintering of Niobium Using Ni–Cu Binders	
2	11:00-11:15	Raj Hans Kumar	Machining Behaviour and Mechanical Properties of High Entropy Alloy	
3	11:15-11:30	Zainul Abedin	Influence of Porosity on Melting Dynamics of Low-Melting Alloy	
4	11:30-11:45	Aman Nigam	Overview of the Role of Mold Fluxes in the Development of 3rd Generation AHSS	
5	11:45-12:00	Antrakrate Gupta	Ceramic slurry dispersion stability assessment technique for DLP 3D printing	
6	12:00-12:15	Aditya Dass	Effect of Alumina in flash reduction of Iron ore fines	
7	12:15-12:30	Pranjal Chauhan	Modeling the effect of powder reuse on meltpool dynamics and defect formation in additively manufactured components	

MATERIAL ADVANTAGE IIT KANPUR

IIM Metallurgy Materials Engineering

MATSOC The Materials Society

Detailed Oral Presentations Schedule

Day:2		Date: 15th March 2026	Slot: Afternoon (15:00 -16:00)	Venue: L18
Technical Sessions-III A: Biomaterials and Bioengineering			Title of Presentation	
Session Chair: Prof. Kantesh Balani				
S.NO	TIME	SPEAKER		
1	15:00-15:15	Dr. Kalpana Rathore	Agar-based Electrospun Bilayer Dressing for Chronic Wound Management	
2	15:15-15:30	Dr. Uma Devi	Biological Evaluation of Phd2 Inducers as Potential Anticancer Agents	
3	15:30-15:45	Murli Manohar	Effect of Feedstock Characteristics on Cell Adhesion, Mineralization, and Nanomechanical Properties of Suspension Plasma-Sprayed Hydroxyapatite/Bioglass Coatings	
4	15:45-16:00	Anupam Halder	Bi2S3 Electrocatalyst for Non-Enzymatic Electrochemical Glucose Detection: Mechanistic Insights and Sensing in Human Blood and Serum	

Day:2		Date: 15th March 2026	Slot: Afternoon (15:00 -16:00)	Venue: L15
Technical Sessions-III B: Modelling and Simulation in Materials Science and Engineering			Title of Presentation	
Session Chair: Prof. Somnath Bhowmick				
S.NO	TIME	SPEAKER		
2	15:00-15:15	Aravind K	Phase-Field–Driven Hybrid Framework with Attention-Enhanced Deep Learning for 2D and 3D Microstructure Evolution in Ternary Alloys	
3	15:15-15:30	Juhi Rani Verma	Crystallization and Heat Transfer Behaviour of Mould Fluxes in Continuous Casting of Peritectic Steel	
4	15:30-15:45	Manish Ranjan	Effect of Ti Addition on Screw-Dislocation Mediated Plasticity in W-Containing Refractory High-Entropy Alloys	
5	15:45-16:00	Rakesh Maurya	Effect of Magnetic Field on Grain Growth in Polycrystalline Materials: A Phase Field Study	

Detailed Poster Presentations

S.NO	Abstract ID	Presenter's Name	Title of Presentation
1	**RSD01**	Neha Maurya	Sustainable Recovery of Metals and Polymers from End-of-life Photovoltaic Modules & Waste Printed Circuit Boards
2	**RSD02**	Aditi Singh Chauhan	Mechanistic Insights into Hydrogen-Metal Interactions in Aerospace-Grade Advanced High-Strength Titanium Alloys
3	**RSD03**	Ayushi Bhatnagar	ZrB2-based Functionally Graded Ultra High Temperature Ceramics for Hypersonic Vehicles
4	**RSD04**	Shivansh	Microstructural and Mechanical characterisation of Additively Manufactured Stainless steel - Mild steel functionally graded material for pipeline application
5	**RSD05**	Shivam Aggarwal	Perovskite TE-Predictor: An Interpretable Machine Learning Framework to Accelerate the Design of Oxide-Perovskite Thermoelectric Materials
6	**RSD06**	Bhumika Sanjay Patankar	Structural Engineering of Doped P2-Type Layered Oxides for High-Stability Sodium-Ion Cathodes
7	**RSD07**	Shruti	High-Entropy Design Strategy for Ultralow Thermal Conductivity in p-Type Oxide Thermoelectric
8	**RSD08**	Kyama Alekhya Kumari	Effect of Solutionizing Duration on Microstructure and Fretting Tribocorrosion Behaviour of AZ91 Mg alloy
9	**RSD09**	Mrinmoy Chanda	Automated sub-grain boundary detection in experimental and synthetic crystal orientation maps of deformed polycrystals
10	**RSD10**	Yash Gupta	Creep life prediction of P91 grade steel using Genetic Algorithms and Physics-Informed Neural Network.
11	**RSD11**	Subhra Khan	Physics-Informed Machine Learning Framework for Magnetic High-Entropy Alloys with Experimental Validation
12	**RSD12**	Pritam Dey	Development of Cost-efficient environmentally friendly thermoelectric materials
13	**RSD13**	Vivek Kumar	High entropy oxides as the next generation high temperature thermoelectric material
14	**RSD14**	Sunraj Patel	Physics-Informed Neural Network for Stress Analysis in In-Plane Crack Problems
15	**RSD15**	Praveen Kumar	PANI-Derived Microporous Activated Carbon with Ultra-High Surface Area for Efficient Removal of Cationic and Anionic Dyes from Wastewater
16	**RSD16**	Kunal Kishore	Performance Analysis of Thermoelectric Generators for Industrial Applications
17	**RSD17**	Saurabh Sharma	Design of Composite Polymer Interface for High-Performance Na-ion Solid-State Batteries
18	**RSD18**	Jeetendra Kumar	Evolution of Quasi-Vertically Oriented Sb2S3 Micropillar Arrays via Sulfurization of Sputtered Antimony Thin Films
19	**RSD19**	Baby Shruit Shukla	Innovative Approaches in Burn Wound Healing: Overcoming Challenges and Advancing Care

Plenary Session:

Decarbonising the steel industry-One molecule at a time

Siddhartha Misra[1]
Chief Process Research, TATA STEEL Jamshedpur, Jharkhand, India[1]

About the Speaker:

Dr. Siddhartha Misra holds a B. Tech. in Materials and Metallurgical Engineering from IIT Kanpur and a MS and Ph D in Materials Science and Engineering from Carnegie Mellon University, Pittsburgh. With over 20 years of professional experience, he is currently working as Chief Process Research at TATA Steel R&D in Jamshedpur. There he is responsible for steering research initiatives in the various facets of iron and steelmaking process. This include utilization of low grade raw materials, advances in coal and coke making and research efforts in the area of sustainability including steel decarbonization, and waste water treatment. His other significant research areas worth mentioning are valorization of steel plant waste. He has also worked in the area of product development, looking at steel grade design, innovative coatings of steel and metal joining and welding. Before moving to R&D, he has worked in various roles focusing on Plant Operations, Quality Assurance and Process Optimization. Prior to shifting bases to India, Dr Misra worked at U. S. Steel Research & Technology Centre in Pittsburgh in the area of steelmaking. An author of over 33 technical papers and book chapters and 10 granted patents, he is the recipient of AIST's Charles H Herty Award, AIST's Hunt-Kelly Outstanding Paper Award and Indian Institute of Metal's Essar Gold Medal and O P Jindal Gold Medal to name a few.

Workshop:

Artificial Intelligence for End-to-End Materials Modelling and Discovery

Anoop Krishnan[1]

Department of Civil Engineering, Indian Institute of Technology Delhi, Delhi, 110016 India[1]

Abstract:

The development of artificial intelligence (AI) systems for scientific discovery presents unique challenges that differ significantly from traditional AI applications. In this talk, we will discuss an end-to-end AI framework that addresses these challenges, using materials discovery as a compelling use case. We will explore how AI approaches can transform a traditionally sequential and time-intensive process into an efficient computational workflow. The discussion will center on a three-tier AI system architecture: (i) specialized large language models (LLMs) and other information extraction models incorporating domain-specific knowledge representations for intelligent search space reduction, (ii) graph neural networks that combine physics-based inductive biases for materials simulation, and (iii) LLM agents for automated experiments. Through practical demonstrations, we will examine how these AI components handle complex scientific problems, particularly focusing on information extraction from tables, generative modeling of crystal structures, and atomistic modeling of materials. We will analyze the integration of physical constraints and domain knowledge into neural architectures, demonstrating how this enhances model interpretability and generalization. The talk concludes by examining open problems in scientific AI, including causal discovery, out-of-distribution generalization, and the seamless integration of symbolic and neural reasoning for scientific applications.

About the Speaker:

Prof. N. M. Anoop Krishnan is an Associate Professor in the Department of Civil Engineering, IIT Delhi with a joint appointment in the Yardi School of Artificial Intelligence. Anoop completed his Ph.D. in Civil Engineering from Indian Institute of Science (IISc), Bangalore in 2015, after which, he worked as a postdoctoral researcher in University of California Los Angeles from 2015 to 2017. Prior to this, he completed his B.Tech. in Civil Engineering from National Institute of Technology Calicut in 2009. He works at the intersection of materials, mechanics, simulations, and AI and ML with the goal of accelerating materials modeling and discovery. He has published more than 120 international peer-reviewed journal publications and has 2 granted patents. He has won several awards including Sir A. Pilkington Award by Society of Glass Technology, UK (2024), Alexander von Humboldt Fellowship (2023) for experienced researchers, Google Research Scholar Award (2023), W. A. Weyl International Glass Science Award by International Commission on Glass (2022), Indian National Academy of Engineering Young Engineer Award (INAE YAE 2020), BRNS-DAE Young Scientist Award (2021), Indian Academy of Sciences Associateship (2022), and National Academy of Science India Young Scientist Award (NASI YSA 2021).

Keynote Lectures:

Sustainable Space Exploration: Air Intakes of Reusable Launch Vehicles

Sanjay Mittal[1]

Department of Aerospace Engineering, Indian Institute of Technology Kanpur, Kanpur, 208016 India[1]

Abstract:

The talk begins with the need for space exploration and the players in the game. Hybrid propulsion systems offer sustainable options for space missions. One such design is to employ a scramjet engine at a certain stage in the flight. Air intakes form a vital component of an airbreathing engine of a aerospace vehicle. We investigate the performance of a mixed-compression intake using stabilized finite element methods implemented on parallel computing platforms. In the sub-critical regime, the normal shock is pushed in the convergent part of the intake leading to the "buzz" instability and "unstart". It adversely affects the mass flow entering the engine and may lead to combustion instability, engine surge and flame out. Little buzz arises due to shear layer instabilities in the intake. Big buzz occurs due to pressure pulses from the subsonic portion of the intake. Flow control techniques such as boundary layer bleed to increase the operational boundaries of these engines are explored. Similar instabilities in intakes of high speed single-engine aircrafts are discussed.

About the Speaker:

Prof. Sanjay Mittal received his undergraduate education in Aeronautical Engineering at the Indian Institute of Technology Kanpur, India. He went to the University of Minnesota, Minneapolis, USA for his graduate education. Presently, he is a Professor in the Department of Aerospace Engineering at Indian Institute of Technology Kanpur, India. His research interests include air-intakes, fluid-structure interactions, flow-induced vibration, bluff body flows, aerodynamic shape optimization, shock-boundary layer interactions, high performance computing, modeling of traffic flow, sports aerodynamics and l ow speed wind-tunnel testing. He is passionate about teaching, and received the Excellence-in- Teaching Award and the Gopal Das Bhandari Distinguished Teacher Award from his Institute. He is a Fellow of the Indian National Academy of Engineering, Indian National Science Academy, Indian Academy of Sciences and National Academy of Sciences. He received the Shanti Swarup Bhatnagar Prize in Engineering Sciences in 2006.

Agar and Cellulose based Dressings for Faster Blood Clotting

<u>Vivek Verma[1]</u>

Department of Material Science and Engineering, Indian Institute of Technology Kanpur, Kanpur, 208016 India[1]

Abstract:

Uncontrolled bleeding from traumatic events such as gunshot wounds, traffic accidents, or war casualties is still one of the primary causes of mortality worldwide. In such an emergency, fast and effective bleeding management is vital to save patient's life. To address this, we have developed an agar-based hemostatic wound cryogels with oxidized cellulose and polydopamine to rapidly arrest bleeding while promoting initial wound stabilization and healing. The cryogel were fabricated using biocompatible and biodegradable polymers offering a porous architecture to support rapid blood absorption, platelet aggregation, and localized coagulation. With a 4200% swelling degree, a quicker clotting time (within 60 s), and a 4.77 kPa compressive strength, the developed hemostatic sponges showed superabsorbent hemostatic activity. In in vitro tests, the cryogels demonstrated outstanding cytocompatibility and hemocompatibility. The developed hemostatic materials exhibited exceptional in vivo hemostatic efficacy in in vivo models attaining blood clotting times of 64 s and 35 s in rat tail amputation and liver puncture models respectively. These findings suggest that the developed hemostatic materials hold strong potential for use in emergency trauma care and battlefield applications, offering a rapid, effective, and scalable solution for hemorrhage control.

About the Speaker:

Dr. Vivek Verma is a faculty of Materials Science and Engineering (MSE) department at IIT Kanpur. He did his B. Tech. in Metallurgical Engineering from IIT Madras and PhD from Pennsylvania State University. His research interests include developing materials for sustainable packaging and wound dressing. His group focusses on physical and chemical modification of polymers. Development of seaweed-based packaging solutions for FMCG products, dressings for chronic wounds, and hemostatic materials for faster blood clotting are few of his contributions. He has filed several patents on packaging and wound care materials. He has been awarded STE Green Excellence Award, Shri Ram Arora Award and American Academy of Mechanics, Founders' Prize and Grant.

Oral Session I A:
Physical and Mechanical Behavior of Materials

Role of Zn addition on microstructural evolution and mechanical properties of a novel Mg-1.2Al-0.4Ca-0.2Ce alloy processed by rotary swaging

Md Irfan Ali[a], Niraj Chawake[a], Srinu Gangolu[a*]
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Abstract

Magnesium (Mg), the lightest structural metal, offers strong potential for automotive and aerospace applications, provided its mechanical properties can be enhanced without heavy rare-earth additions or complex processing routes. Here, Mg-1.2Al-0.4Ca-0.2Ce-xZn alloy with varying Zn content (0.4%, 0.8%, 1.6%) was prepared by room temperature rotary swaging, imparting the same amount (26%) of plastic strain in all the three alloys. The three as-swaged alloys exhibit heterogeneous microstructures consisting of twin-rich coarse grains, shear-band regions containing fine grains, and relatively undeformed large grains. The investigation confirms grain refinement is governed by the synergistic effects of twinning, shear banding, and dislocation-driven sub grain formation mechanism. It also confirms fragmentation of the Laves phases and their uniform distribution after rotary swaging. Increase in Zn addition caused consistent decrease in average grain size due to its role on improving efficiency of grain subdivision mechanisms namely twinning, shear banding, sub grain formation mechanism by suppressing twin thickness, accelerating shear band assisted grain subdivision and activation of non-basal slip respectively. Also, rotary swaging caused texture heterogeneity in the microstructure, showing (0001) // swaging direction (SD) in the fine grains inside shear bands and (10-10) // SD in the twin rich coarse grains and relatively undeformed large grains. Rotary swaging improves both yield strength and tensile strength with increased Zn without sacrificing ductility (4.48%, 7.8%, 5.32%). Yield strength increases from 153 MPa to 176 MPa to 200 MPa and tensile strength increases from 202 MPa to 284 MPa and then slightly decreased to 248 MPa with increased Zn content (0.4%, 0.8%, 1.6%). The improvement in mechanical properties with increase in Zn is mainly attributed to heterogeneous bimodality in both microstructure and texture assisted by grain refinement, dislocation strengthening and second phase strengthening.

Keywords: Rotary swaging, Microstructural evolutions, Mechanical properties, Heterogeneous microstructures, Basal texture.

Interface-Controlled Creep in a Non-Equiatomic CoCrNi Alloy with Hierarchical Microstructure

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Abstract

High temperature deformation in heterogeneous alloys is inherently complex, as distinct microstructural constituents may deform through different rate-controlling mechanisms, including viscous glide and dislocation climb, diffusion-assisted processes, grain-boundary sliding, and interface-mediated deformation. The concurrent operation of these mechanisms complicates the identification of a unique governing process and necessitates a microstructure-sensitive framework for mechanistic interpretation. In the present work, we investigate the creep behaviour of a novel non-equiatomic CoCrNi alloy exhibiting a hierarchical microstructure composed of an fcc γ matrix, a bcc β phase, and nanoscale precipitates embedded within the β phase. Systematic compressive creep experiments were conducted in the temperature range of 600–750°C and stress varying from 100 – 200 MPa. At lower temperatures (600–675°C), creep deformation is dominated by dislocation-controlled hardening, and a steady-state regime is not attained. In contrast, at higher temperatures (700–750°C), a steady-state regime emerges due to a dynamic balance between dislocation hardening and softening via recovery and recrystallisation. A comprehensive microstructural assessment, utilizing electron backscatter diffraction (EBSD) and transmission electron microscopy (TEM), was carried out on crept samples to explore the micro-mechanisms and elucidate the role of hierarchical phase structure during creep. Based on the insights of characterised defect structure within phases, multiple creep models are employed to rationalise the governing deformation mechanism and predict steady-state strain rates in this hierarchical alloy system. This study establishes a mechanistic framework for understanding creep in multiphase alloys and provides guidance for the design of high-temperature-resistant heterogeneous materials.

Keywords: Hierarchical Microstructure, Creep, Dislocations, Dynamic Recrystallisation.

Connectivity-Based Grain Boundary Engineering of FeCoCrNiMn High Entropy Alloy: Effect of Deformation and Annealing on CSL Network Evolution and Corrosion Behaviour

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Abstract

High Entropy Alloys (HEAs) are a new class of material made by mixing several main elements in almost equal amounts, instead of having one primary element like in traditional alloys. Among them, the FeCoCrNiMn (Cantor alloy) exhibits a stable single-phase FCC structure and low stacking fault energy, which promotes the formation and regeneration of twins during deformation and annealing. These characteristics make it an excellent candidate for Grain Boundary Engineering (GBE). Grain boundaries play a crucial role in controlling the mechanical and corrosion properties of materials. Special Coincidence Site Lattice (CSL) boundaries such as Σ3 (annealing twins) have low interfacial energy and improved resistance to degradation. In the present work, Grain Boundary Engineering was carried out on the Cantor alloy through controlled cold rolling (8%, 15%, 30%, and 45%) followed by annealing at different temperatures for 60 minutes under non-iterative processing conditions. The evolution of the Grain Boundary Character Distribution (GBCD) was systematically analysed using both conventional and connectivity-based parameters. In addition to CSL length fractions and Σ3 fractions, advanced network descriptors were employed, including Twin Related Domains (TRDs), Longest Length Chain (LLC) based on percolation theory, correlation length, and triple junction (TJ) ratio. Network-weighted LLC and correlation length were used to quantify CSL connectivity, while the TJ ratio ((J2+J3)/ (J0+J1)) was used to evaluate local junction strengthening. The results indicate that strain recrystallization is prominent at higher deformation levels (30% and 45%) across all annealing temperatures. In contrast, moderate deformation levels (8% and 15%) followed by annealing at temperatures above 950 °C produce the most effective Grain Boundary Engineering response. Moderate strain promotes strain-induced boundary migration and twin regeneration, leading to improved CSL connectivity, strengthening of triple junctions, and effective fragmentation of the random high-angle grain boundary network. Corrosion studies performed in 0.5M H_2SO_4 and 0.6M NaCl environments further revealed that microstructures with improved CSL connectivity and higher triple junction ratios exhibit enhanced resistance to localized attack, with Σ3 and Σ9 boundaries showing greater immunity to pitting compared to random high-angle grain boundaries. Overall, this study demonstrates that optimized low-to-moderate deformation followed by appropriate annealing significantly enhances CSL boundary fraction, network connectivity, and triple junction strengthening in the Cantor alloy. Connectivity-based metrics are very important in Grain Boundary Engineering and provides a practical pathway to improve both structural and corrosion performance of FCC high entropy alloys.

Keywords: Grain Boundary Engineering (GBE), Twin Related Domains (TRDs), Grain Boundary Character Distribution (GBCD), Coincidence Site Lattice (CSL) Boundaries.

Investigating Interdiffusion in B2 (Ni, Ru) Al Alloy

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Abstract

Bond coats are critical constituents of multilayer thermal barrier coating (TBC) systems, typically composed of the B2 (Ni,Pt)Al phase. However, the dependence on Pt significantly increases the cost of these coatings. A promising approach to reduce the overall cost is the partial or complete replacement of Pt with Ru. For the design and optimisation of Ru-based bond coats, it is essential to understand the interdiffusion behaviour of the (Ni,Ru)Al system. In the present work, diffusion in the single B2 phase of the Ni-Al-Ru system was investigated at 1100 °C using the diffusion couple technique. Experimental concentration profiles were obtained using an Electron Probe Micro Analyser, which were subsequently analysed with the ***MultiDiflux*** software. In this study, interdiffusion behaviour is presented in terms of concentration gradients, interdiffusion fluxes, and interdiffusion coefficients. Furthermore, the analysis is extended to evaluate the interdiffusion coefficients in both the volume-fixed and mass-fixed frames of reference, highlighting the significance of reference frame selection in multicomponent diffusion. In addition, the influence of molar volume variation on the calculated interdiffusion coefficients is discussed.

Keywords: Interdiffusion, Bond coats, Concentration profiles.

Microstructure and Mechanical Property Correlation in High-Entropy Dual-Phase (Ti, Zr, Ta, Hf) Boride-Carbide-Based Ultra High Temperature Ceramic

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Abstract

Ultra-High Temperature Ceramics (UHTCs), particularly the borides and carbides of Zr, Ti, Ta, and Hf, are promising candidates for extreme environments owing to their extremely high melting points (>3000 °C). This study developed a (Zr, Ti, Ta, Hf)-based dual-phase high-entropy boride–carbide (HEB–HEC) ceramic and a 20 vol.% SiC-reinforced HEB–HEC composite to achieve a refined microstructure and improved mechanical properties compared with single-phase HEB and HEC. All compositions - (i) HEB, (ii) HEC, (iii) HEB–HEC, and (iv) HEB–HEC–SiC were consolidated using Spark Plasma Sintering (SPS) at 2000 °C under 40 MPa for 30 min, resulting in near-theoretical densities (~99%). Phase analysis confirmed the formation of single-phase solid solutions in both HEB and HEC. In contrast, the dual-phase HEB–HEC composite consisted of ~51 vol.% boride and ~49 vol.% carbide phases, whereas the HEB–HEC–SiC composite comprised ~40 vol.% HEB, ~41 vol.% HEC, and ~19 vol.% SiC. Microstructural analysis revealed that the presence of secondary phases effectively inhibited grain growth through a pinning effect, significantly reducing the grain size from 5.6 µm in single-phase HEB to 1.1 µm in the SiC-reinforced composite. This microstructural refinement resulted in a notable mechanical synergy. The dual-phase HEB–HEC composite exhibited a flexural strength of ~595 MPa and a fracture toughness of ~4.1 MPa $m^{1/2}$, while the SiC-reinforced composite demonstrated superior overall performance, achieving a flexural strength of ~580 MPa, fracture toughness of ~4.9 MPa $m^{1/2}$, and microhardness of ~27.3 GPa. These results demonstrate that SiC-reinforced high-entropy dual-phase UHTCs provide an effective pathway for enhancing the mechanical performance of UHTCs, making them promising materials for demanding aerospace and hypersonic applications.

Keywords: High-Entropy Ceramics; Dual-Phase UHTCs; Spark Plasma Sintering; Zener Pinning; Mechanical Properties.

Oral Session I B:
Extractive Metallurgy and Corrosion of Metals

Enrichment of Lean-grade Iron Ores using Reduction Roasting for Sustainable Ironmaking

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Abstract

India is the second-largest steel producer globally, with an annual crude steel output of ~150 million tonnes in 2024. The integrated blast furnace basic oxygen furnace (BF–BOF) route remains the dominant production technology. Although highly efficient, this route is energy-intensive and a major source of CO_2 emissions. On average, crude steel production worldwide emits ~1.9 tonnes of CO_2 per tonne, accounting for nearly 8% of global emissions. In India, the emission intensity is significantly higher (~2.5 tonnes of CO_2 per tonne of crude steel), largely due to the inferior quality of raw materials. For BF-based iron making, a prepared burden in the form of high-quality agglomerates is essential, which is itself an energy-intensive process. However, the rapid depletion of high-grade iron ore has made this increasingly challenging. With India targeting 300 million tonnes of crude steel production by 2030, the effective utilisation of lower-grade ores is critical. This study investigates the enrichment of lean-grade ores through reduction roasting, employing both conventional and novel process routes. It is observed that full conversion of BF raw material from hematite to magnetite can reduce CO_2 emissions by ~104 kg per tonne of hot metal and lower coke consumption by ~35 kg. Particular emphasis is placed on the use of alternative reducing agents such as biomass and gaseous hydrogen, with the objective of lowering CO_2 emissions associated with enrichment processes.

Keywords: Iron ores, Roasting, Environmental protection.

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Reduction Behaviour of Hematite Concentrates in a Hydrogen-Based Flash Ironmaking Reactor

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Abstract

The reduction kinetics of hematite concentrates were investigated in a flash ironmaking reactor over a temperature range of 900–1100 °C in a pure hydrogen atmosphere. A global rate law was formulated to describe the reduction of hematite concentrates in a hydrogen atmosphere. The results indicate that the reduction of hematite concentrate particles is governed by a nucleation-and-growth mechanism, characterised by an Avrami exponent of n=2. The kinetic parameters, namely the activation energy and the pre-exponential factor, were determined to be 37.496 kJ/mol and 50.263, respectively, for describing the reduction behaviour in a hydrogen environment. An increase in temperature led to an enhanced reduction rate, whereas an increase in particle size resulted in a significant decrease in the reduction rate. This reduction was primarily attributed to the decrease in particle residence time, which reduced the effective gas–solid contact time within the reaction tube. Both experimental and modelling results showed that, for particle sizes larger than 100 μm, variations in the gas flow rate have only a limited effect on particle residence time within the range of operating conditions investigated. The global rate law was incorporated into a particle-scale model to solve the mass transfer equations governing the reduction process. The model was used to predict particle velocity, particle temperature, and degree of reduction along the reactor length, providing a detailed evaluation of particle heating behaviour and residence time within the flash ironmaking reactor.

Keywords: Hematite concentrates, hydrogen, Flash Ironmaking reactor, Temperature Sustainability.

Hydrogen Production through Recycling of Black Aluminium Dross via Alkaline Leaching

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Abstract

The increasing generation of aluminium dross as a by-product of primary and secondary aluminium industries presents significant environmental challenges while simultaneously offering opportunities for resource recovery. Nearly 8 wt.% of the total aluminium produced is converted into dross, making its effective recycling an important area of research. The present study investigates the recycling of black aluminium dross as a secondary resource for hydrogen generation through alkaline leaching. In this work, the aluminium present in black dross reacts with water in the presence of alkaline reagents such as sodium hydroxide (NaOH) and potassium hydroxide (KOH), which facilitates hydrogen evolution. A certain quantity (2 g) of ground black aluminium dross was reacted with alkaline solutions of varying molarities (0.25-1 M) at different temperatures (30-60 °C) under continuous agitation of 400 rpm to enhance the reaction kinetics. Under optimised conditions, hydrogen volumes of approximately 330 mL were obtained, and the reaction proceeded rapidly during the initial stage before gradually approaching completion within approximately 30 minutes. Kinetic analysis revealed that the Avrami-Erofeyev model provided the best fit to the experimental data, with calculated activation energy values of 66.7 and 64.7 kJ/mol for the NaOH and KOH systems, respectively. The results demonstrate the potential of recycling black aluminium dross through hydrometallurgical treatment for hydrogen generation under relatively mild conditions. This approach provides a viable pathway for the valorisation of aluminium industry waste while contributing to sustainable resource utilisation and cleaner process development.

Keywords: Black dross, Hydrogen generation, Hydrometallurgy, Recycling, Waste Management.

Effect of Pseudomonas aeruginosa on corrosion behaviour of Mild Steel in Marine Environment

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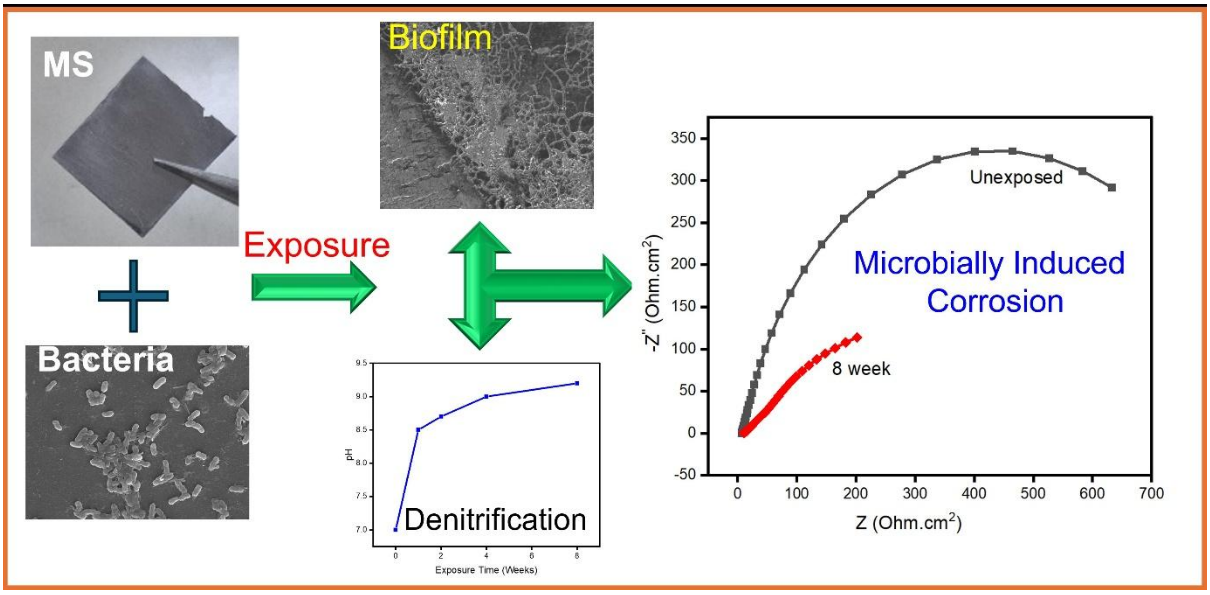
Abstract

Mild steel is prone to biofouling and microbially induced corrosion. Owing to its extensive use in the marine industry, it is of paramount importance to comprehend various metal-microbe interactions leading to microbially induced corrosion and thus control their catastrophic failures. Being gram-negative bacteria and facultative anaerobes, Pseudomonas aeruginosa are widely implicated in premature failures of steel due to their tendency to form biofilms on the steel surface. These biofilms can modify the corrosion behaviour of the steel. Mild Steel samples were exposed to microbial growth environment (LB media) containing the bacteria for different periods of time, namely 1 Week, 2 Week, 4 Week and 8 Week. SEM analysis and corrosion tests, such as Open circuit potential analysis, electrochemical impedance spectroscopy, linear polarisation resistance and tafel test, were performed to understand the underlying corrosion mechanism for microbially induced corrosion and biofilm characteristics. There was a significant biofilm on the steel surface, leading to about 6 times increase in the corrosion rate of the 8-week exposure sample compared to the unexposed mild steel. This could be attributed to the formation of biofilm and denitrification as indicated by the increase in the pH of the microbial growth media. Equivalent circuit modelling of the impedance data revealed that the heterogeneous nature of biofilms was responsible for the observed deterioration of corrosion resistance of the steel.

Keywords: Bio fouling, Corrosion, Steel, Pseudomonas aeruginosa, Electrochemical impedance spectroscopy.



In-situ investigation on hydrogen-induced deformation micro mechanisms in commercially pure titanium

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Abstract

The transition toward a hydrogen-based energy infrastructure has intensified concerns regarding hydrogen embrittlement and its impact on the mechanical reliability of structural alloys. Titanium and its alloys are attractive for hydrogen-related applications due to their high specific strength, corrosion resistance, and low density; however, prolonged exposure to hydrogen-rich environments can significantly degrade their mechanical performance. Despite extensive studies on titanium alloys, the fundamental deformation micro mechanisms of hexagonal close-packed α-titanium in the presence of hydrogen remain insufficiently understood. In this work, hydrogen-assisted deformation behaviour of commercially pure titanium was investigated under uniaxial tensile loading. Electrochemically hydrogen-charged specimens were homogenized at 573 K to ensure uniform hydrogen distribution and tested at a strain rate of 10^{-3} s^{-1}. Hydrogen charging increased yield strength and ultimate tensile strength, while the uniform elongation decreased by nearly 40 percent. 2D digital image correlation revealed pronounced strain localization in hydrogen-charged samples. Fractographic analysis showed a transition from ductile dimple rupture to quasi brittle fracture associated with hydride formation along grain boundaries. In situ SEM-EBSD tensile experiments demonstrated that hydrogen suppresses prismatic slip while promoting deformation twinning and pyramidal ⟨c+a⟩ slip. Hydride precipitation increased the stress required for twin activation, promoted localized twin nucleation, and inhibited twin thickening. Post-necking deformation in hydrogen-charged specimens was sustained through localized twinning and crack-tip blunting, resulting in only a limited reduction in total strain. The influence of crystallographic texture and microstructural anisotropy on hydrogen-induced deformation and fracture mechanisms in commercially pure titanium will be discussed.

Keywords: Hydrogen-induced deformation, Fracture mechanisms, Microstructural anisotropy.

Oral Session II A:
Functional and Energy Materials

Cold sintering–assisted microstructural engineering of $Na_{3.2+x}Zr_{2-x}Mg_xSi_{2.2}P_{0.8}O_{12}$ solid electrolytes enabling enhanced Na-metal battery performance

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Abstract

The cold sintering process (CSP) has emerged as an energy-efficient densification strategy for ceramic materials, enabling microstructural consolidation at reduced thermal budgets. Conventional sintering of NASICON-type solid electrolytes typically requires high temperatures (≥1250 °C), which often leads to sodium and phosphorus volatilisation, secondary phase formation, and degradation of interfacial electrochemical stability. $Na_3Zr_2Si_2PO_{12}$ (NZSP), a promising solid electrolyte for sodium-ion batteries, is particularly sensitive to such high-temperature processing. In this work, CSP-assisted densification of magnesium-doped NZSP is systematically investigated and benchmarked against conventionally sintered NZSP processed at 1250 °C (CS-1250). Dense electrolyte pellets were successfully obtained at a reduced sintering temperature of 1150 °C using CSP. X-ray diffraction and scanning electron microscopy reveal that CSP induces a distinct microstructure with improved grain connectivity and reduced residual pores compared to CS-1250 samples. Electrochemical impedance spectroscopy confirms comparable ionic conductivity despite the lower processing temperature. The influence of CSP-induced microstructure on interfacial stability was evaluated using Na|NZSP|Na symmetric cells. CSP-processed electrolytes exhibit markedly improved Na plating/stripping stability and lower interfacial polarisation compared to CS-1250, indicating enhanced Na-electrolyte compatibility. Furthermore, sodium-metal cells assembled with iron-doped $Na_3V_2(PO_4)_3$ (NVFP) as the cathode demonstrate stable cycling behaviour, achieving ~89% capacity retention over 100 cycles at a C/8 rate. These results establish cold sintering–assisted microstructural engineering as an effective strategy to simultaneously reduce processing temperature and enhance interfacial and electrochemical performance in NASICON-type solid electrolytes.

Keywords: Cold Sintering Process, Na-ion Battery, NASICON.

Hierarchically Engraved $NiFePO_4$ Microrods on MWCNTs for Next-Generation Scalable Supercapacitor Electrodes

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Abstract

The quest for sustainable, cost-effective, and scalable supercapacitor electrodes persists as a critical barrier to widespread energy storage adoption. By synergistically combining the rich redox chemistry of phosphate frameworks with the exceptional conductivity of carbon nanotube networks, we present a breakthrough binder-free electrode architecture. Through a straightforward two-step chemical strategy, highly porous rectangular $Ni_3Fe_4(PO_4)_6$ microrods are directly engraved onto multi-walled carbon nanotube (MWCNT) backbones, creating a robust, interconnected, and hierarchically porous hybrid structure. Comprehensive structural and morphological characterisations reveal a pure triclinic phosphate phase, strong interfacial bonding, and abundant nanoscale porosity. Electrochemical evaluations via cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS) further corroborated by a large-area (10 cm × 4 cm) symmetric device demonstrate outstanding performance: a remarkable specific capacitance of 2226 F g^{-1} (1 F cm^{-2}) at 5 mV s^{-1}, excellent rate capability, and 82% capacitance retention after 2000 cycles. The assembled device delivers an energy density of 26 Wh kg^{-1} at a power density of 526 W kg^{-1}, with stable long-term operation. Notably, the prototype successfully powers a 1 V DC fan, highlighting its practical viability. This work introduces a scalable, eco-friendly phosphate–carbon hybrid platform that bridges advanced materials design with real-world supercapacitor applications, paving the way for next-generation energy storage solutions.

Keywords: Nickel–iron phosphate; MWCNT composite; Porous microrods; Binder-free electrode; Supercapacitor device; Electrochemical energy storage.

Investigating partial oxidation of CH_4 in CO_2-rich environments using $Gd_{0.1}Ce_{0.9}O_{2-\delta}$–$SrFe_{0.9}Ti_{0.1}O_{3-\delta}$ composite oxygen transport membranes

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Abstract-

Oxygen-transport membranes enable compact reactors for syngas generation by supplying distributed oxygen to methane at high temperatures. In this work, we investigate Ni and Co free partial oxidation of methane in CO_2-rich atmospheres using a dense $Gd_{0.1}Ce_{0.9}O_{2-\delta}$ –$SrFe_{0.9}Ti_{0.1}O_{3-\delta}$ (GDC–SFTO) composite membrane with porous functional layers of the same composition on both sides. With 0.21 O_2/0.79 Ar as the feed and CH_4/CO_2 mixtures as the permeate side, the membrane exhibits strong reaction-enhanced permeation, reaching ~6-7 mL.cm^{-2}.min^{-1} at 950 °C (0.4–0.5 mm thick dense layer with ~32 µm porous coatings), and maintains stable flux during extended operation at 900°C. Systematic variation in methane partial pressure reveals an increase in flux followed by saturation, while methane conversion declines from ~99% to ~20% as oxygen delivery becomes limiting. Electrochemical impedance spectroscopy of the symmetric cells using GDC-SFTO electrodes, analysed using a transmission-line framework, shows that methane strongly accelerates interfacial oxygen exchange/consumption (rspCH4-0.6), while the porous transport resistance shows only a weak dependence on gas composition. The apparent activation energy of flux at 0.2 CH_4/0.8 CO_2 (~142 kJ·mol^{-1}) matches that of the surface resistance (~148 kJ·mol^{-1}), demonstrating that surface processes dominate reactive permeation in the catalyst-free regime. The combined permeation–reaction–impedance analysis provides a quantitative benchmark for catalyst-free operation and identifies operating windows that maximize oxygen delivery while mitigating degradation in CH_4/CO_2 mixtures.

Keywords: Oxygen transport membranes, environmental protection.

Tuneable insulator–metal transition in epitaxial VO_2 thin films via strain and defect engineering

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Abstract

The Metal to Insulator Transition (MIT) in materials, particularly vanadium dioxide (VO_2), has garnered significant research interest due to its potential applications in smart windows, memristors, transistors, sensors, and optical switches. The transition from an insulating, monoclinic phase to a conducting, tetragonal phase involves changes in optical and electrical properties, opening avenues in adaptive radiative coolers, optical memories, photodetectors, and optical switches. VO_2 exhibits MIT close to 68 °C, thereby requiring tuneable transition temperatures (T_c) in VO_2 thin films for practical device applications. In this work, we explore the role of strain and defect engineering in tuning the MIT temperature in epitaxial VO_2 thin films deposited on c-cut sapphire using Pulsed Laser Deposition (PLD). The study involves tuning the metal-to-insulator transition (MIT) by varying growth parameters, mainly temperature and oxygen partial pressure. Strain engineering along the b-axis helped tune the transition temperature from 65 °C to 82 °C with the out-of-plane b-strain varying from −0.71% to −0.44%. Comprehensive structural and property analyses, including X-ray diffraction (XRD), Reciprocal Space Mapping (RSM), X-ray Photoelectron Spectroscopy (XPS), Raman spectroscopy, and resistivity– temperature (R–T) measurements, were performed to correlate structural properties with T_c. Additionally, density functional theory (DFT) calculations were performed using Quantum Espresso within the generalized gradient approximation of the revised Perdew–Burke–Ernzerhof (PBEsol) functional to provide theoretical validity to the experimentally obtained results. Our study provides critical insights into the interplay between strain and oxygen vacancies and their effect on the physical properties of VO_2 thin films with DFT calculations supporting the experimental findings.

Keywords: thin films, epitaxy, density functional theory, strain engineering, defect engineering.

Synergistic Enhancement of Lithium-Sulfur Battery Performance via a Sugarcane Bagasse Derived Porous Carbon Sulfur Cathode and a Bi_2Se_3 Catalytic Interlayer

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Abstract

Lithium–sulfur (Li–S) batteries have emerged as promising next-generation energy storage systems owing to their high theoretical specific capacity (1675 mAh/g) and low material cost. However, their practical implementation is hindered by rapid capacity fading and limited cycle life, primarily caused by the polysulfide shuttle effect, significant volume expansion during cycling, and the intrinsically poor electrical conductivity of sulfur and its discharge products.

In this work, we present a synergistic design strategy that integrates a sugarcane bagasse-derived porous carbon cathode host with a catalytic Bi_2Se_3-modified separator to overcome poor conductivity and polysulfide shuttle effects. Activated carbon derived from sugarcane bagasse was utilised as a high-surface-area, conductive sulfur host, facilitating effective sulfur encapsulation and buffering of volumetric expansion. To further suppress polysulfide diffusion, a polar and conductive Bi_2Se_3 interlayer was coated onto a polypropylene separator. The Bi_2Se_3 layer provides strong chemical affinity toward lithium polysulfides and promotes their catalytic redox conversion, thereby mitigating the shuttle effect and improving sulfur utilisation. The assembled Li–S cell exhibits an initial specific capacity of ~1100 mAh/g and retains ~54.5% of its capacity after 300 cycles at a C/10 rate. In contrast, the cell without the Bi_2Se_3 interlayer delivers an initial capacity of ~800 mAh/g but retains only ~47.5% after 300 cycles at a C/10 rate. Overall, this study demonstrates a sustainable and effective approach that combines biomass-derived carbon architecture with catalytic interlayer engineering to realise high-performance and durable Li–S batteries.

Keywords: Polysulfide shuttling, Li-S Battery, Layered Materials, Interlayer engineering.

Sintering Kinetics of Nano Al_2O_3 - 3 mol% Y_2O_3-stabilized ZrO_2 Composites during Intermediate and Final Stages via Spark Plasma Sintering

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Abstract

Nanostructured oxide coatings undergo sintering during deposition and high-temperature exposure. This continued densification strongly affects microstructure development and, in turn, long-term mechanical properties and coating lifetime. Understanding nano-powders consolidation under realistic thermal and pressure conditions is therefore critical. Spark plasma sintering (SPS), with its rapid heating rates (100 °C·min^{-1}), serves as a practical method for simulating the fast, non-equilibrium sintering conditions typical of advanced nanocomposite thermal barrier coatings (TBCs). In this study, pure α-Al_2O_3 and Al_2O_3-3 mol% Y_2O_3-stabilized ZrO_2 (3YSZ) composites were consolidated via SPS at 50 MPa over the temperature range 1200–1550 °C. Relative density and grain size are evaluated to elucidate the underlying mechanisms of densification and coarsening. Intermediate-stage densification in pure Al_2O_3 is dominated by grain-boundary diffusion (stress exponent ~ 2). This mechanism persists as the rate-controlling step in the Al_2O_3-3YSZ composite (A3Y), although the effective temperature shifts upward by 100–150 °C. The apparent activation energy for densification increases significantly from 238 kJ·mol^{-1} in monolithic Al_2O_3 to ~429 kJ·mol^{-1} in A3Y, reflecting strong retardation of grain-boundary transport caused by the uniform dispersion of nano 3YSZ particles. Grain-growth kinetics analysis yields activation energies of ~ 590 kJ·mol^{-1} for pure Al_2O_3 (lattice-diffusion control) and ~424 kJ·mol^{-1} for A3Y. The second-phase 3YSZ inclusions reduce the grain-boundary velocity by approximately one order of magnitude via Zener pinning, thereby substantially suppressing coarsening at high temperatures. Thus, highlights the superior microstructural stability and high-temperature mechanical integrity of Al_2O_3-3YSZ composites compared with pure Al_2O_3, positioning the composite as a promising candidate for next-generation thermal barrier coating systems in gas-turbine applications.

Keywords: Densification mechanisms, Spark Plasma sintering, Al_2O_3, 3YSZ.

Oral Session II B:
Materials Processing

Liquid Phase Sintering of Niobium Using Ni–Cu Binders

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Abstract

Niobium (Nb) is a refractory metal of considerable technological importance. However, its consolidation through conventional solid-state sintering remains challenging due to its low solid-state diffusivity, strong affinity for interstitial impurities, and the need for very high processing temperatures. Liquid phase sintering (LPS) presents a potential alternative route to overcome these limitations by introducing a transient liquid phase to enhance mass transport during sintering. In the present work, the feasibility of liquid phase sintering of Nb using Ni–Cu binder systems are examined. The selection of Ni–Cu binder compositions, sintering temperatures, and processing parameters is guided by CALPHAD-based thermodynamic calculations performed under both equilibrium and non-equilibrium conditions. These calculations are employed to identify liquid formation ranges, phase stability, and phase evolution during heating and cooling in the Nb–Ni–Cu system. The presence of liquid enhances mass transport through solution–precipitation mechanisms, thereby promoting accelerated densification at temperatures significantly lower than those required for solid-state sintering of Nb. Compared to conventional Nb sintering carried out at 1900–2100 °C, the proposed approach aims to achieve effective densification in the temperature range of 1400–1500 °C, with reduced sintering times and improved process efficiency. The use of Ni and Cu binders is motivated by their ability to form liquid phases at low temperatures (1100-1400 °C), facilitate rapid pore elimination, and improve microstructural homogeneity while remaining compatible with Nb-based systems. The anticipated outcomes include near-theoretical densification, refined and refined and more uniform microstructures, reduced oxygen pick-up due to shorter high-temperature exposure, and improved processing efficiency. This work establishes a thermodynamically guided framework for liquid phase sintering of Nb and forms the basis for systematic experimental investigations on phase evolution, microstructural development, and optimisation of properties for high-temperature applications.

Keywords: Liquid phase sintering, Microstructure development.

Machining Behaviour and Mechanical Properties of High Entropy Alloy

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Abstract:

High Entropy Alloys (HEAs) are a class of metallic materials composed of at least three principal elements, each with atomic concentrations typically ranging from 5 to 35 at.%. The presence of multiple major elements results in high configurational entropy, which stabilizes simple solid solution phases such as BCC, FCC, and HCP. HEAs are known for their exceptional mechanical properties, which remain stable across a wide temperature range—from cryogenic levels up to ultra-high temperatures (≥2500 °C). This makes them suitable for critical applications, including turbine blades, heat shields, and structural components in jet engines and space vehicles. To achieve the desired shape and dimensions for such applications, machining of HEAs is essential. This seminar focuses on the machining behavior and microstructural evolution of post-machined HEAs. Due to the severe lattice distortion caused by the presence of multiple principal elements, dislocation motion is hindered, leading to enhanced yield strength and ultimate tensile strength (UTS). Since UTS is directly proportional to hardness, HEAs are inherently difficult to machine efficiently.

Over the past five years, researchers worldwide have extensively investigated the machining behavior of High Entropy Alloys (HEAs), focusing particularly on equiatomic and non-equiatomic Cantor alloys (e.g., $Co_{15}Cr_{25}Fe_{20}Mn_{25}Ni_{15}$) and refractory HEAs (e.g., HfZrTiTaAl). These alloys, known for their exceptional hardness and strength, pose significant challenges during machining, such as high cutting forces, rapid tool wear, and difficulty in material removal. In parallel, optimization of machining parameters using multi-criteria decision-making methods such as Taguchi and TOPSIS has shown promise in improving performance. Advanced characterization tools including XRD, SEM, TEM, have been employed to study microstructural evolution of machined surfaces, while mechanical properties are assessed through tensile testing, fracture toughness evaluation, micro-hardness, and nano-indentation.

Keyword: High Entropy Alloys, Microstructure evolution.

Influence of Porosity on Melting Dynamics of Low-Melting Alloys

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Abstract

This study investigates the melting behavior of Wood's metal alloy, emphasizing the role of controlled porosity in cast samples through a combined experimental and numerical approach. Experimentally, porosity was incorporated by drilling the as cast sample as per the calculations for porosity dimensions. The alloy sample was melted using a centrally positioned electric resistance heating rod within a cylindrical chamber under precisely controlled thermal and electrical conditions. Initially, heat conduction dominated, with melting starting near the rod, followed by intensified natural convection in the molten regions, causing temperature stratification. The effects of porosity, heating power, insulation, and heating element depth were systematically explored. Results showed that higher porosity introduces thermal resistance, delaying heat transfer and reducing melting rates, while increased heating power and deeper rod placement enhanced efficiency.
To complement these findings, a numerical model was developed using Ansys-Fluent, employing the enthalpy-porosity method to simulate phase change and natural convection with similar boundary conditions. The model elucidated temperature distributions, melt front progression, and porosity's impact on heat transfer mechanisms, predicting that lower porosity accelerates phase transitions, while insulated boundaries improve thermal efficiency by minimizing heat loss. The integrated experimental-numerical approach confirmed that porosity significantly governs melting dynamics, with higher levels impeding progress due to reduced conductivity. This study provides a validated framework for optimizing melting processes of porous mass.

Keywords: Wood's metal melting; porous scrap; melting dynamics; numerical modelling; experimental validation.

Overview of the Role of Mold Fluxes in the Development of 3rd Generation AHSS

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Abstract

Mold fluxes play a crucial role in the continuous casting of steel by providing lubrication between the copper mold and the solidifying steel shell while also controlling heat transfer from the steel to the mold. The efficiency of these functions strongly depends on the thermophysical properties and crystallization behavior of the slag film formed during casting. Heat transfer across the mold–shell interface is primarily governed by the structure and crystallinity of the slag film (f_{crys}/relative crystallinity), whereas lubrication mainly depends on the viscosity of the mold flux. Advanced High Strength Steels (AHSS) are increasingly being developed for automotive applications due to their superior strength-to-weight ratio, which improves vehicle crashworthiness and fuel efficiency. These improved properties are achieved through the addition of alloying elements such as Al (1–2 wt.%) and manganese (6–7 wt.%). However, conventional CaO–SiO_2 based mold fluxes react with the high Al and Mn content of these steels, leading to interfacial reactions that alter the composition and properties of the mold flux. These reactions can cause unstable heat transfer and casting defects, such as surface defects, and sometimes lead to breakouts. To address these challenges, the present work focuses on the development of non-reactive CaO–Al_2O_3 based mold fluxes suitable for casting high-Al medium-Mn steels belonging to the 3rd generation AHSS family. The effect of varying the w(CaO)/w(Al_2O_3) ratio on crystallization behavior and key thermophysical properties, including viscosity and melting temperature, is investigated. At the end, a numerical model with coupled heat transfer and fluid flow phenomena across the mold–shell interfacial gap is evaluated using the thermophysical properties of the slag film. The model was calibrated through the industrial data. This will give the prediction of various parameters related to the continuous casting of any grade of steel.

Keywords: Mold Flux; Crystallization; Viscosity; Melt Structure; Heat Transfer.

Ceramic slurry dispersion stability assessment technique for DLP 3D printing

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Abstract

Ceramic-loaded aqueous and non-aqueous slurries often exhibit inhomogeneities that lead to non-uniformity, phase separation, and unstable dispersion. In vat photopolymerization–based 3D printing, crosslinking unstable ceramic suspensions results in non-uniform ceramic distribution, causing structural defects and geometric deviations in printed parts. This work presents a pixel-tracking–based characterization methodology utilizing computer vision and image processing to evaluate slurry stability. The algorithm identifies localized pixel intensity variations arising from density fluctuations within the slurry and quantifies dispersion stability over time. The developed method was applied to 15 formulations of hydroxyapatite-loaded aqueous slurries, varying particle size (10 µm, 300 nm, 200 nm, and 100 nm), solid loading (5, 10, and 12 vol%), and dispersant content (0, 2, 4, and 6 wt%). For proof of concept, 10 vol% hydroxyapatite-loaded non-aqueous photopolymer slurries were printed into 10 × 10 × 10 mm^3 polymer-ceramic scaffolds (0.5 mm strut size with 2 mm square pores) using digital light processing (DLP). Improved slurry stability mitigated spatial inhomogeneity and reduced undesired geometric and compositional variations in the printed composite scaffolds. These results highlight the importance of quantitative slurry characterization in minimizing experimental iterations, accelerating formulation optimization, and eliminating pseudo-stable compositions.

Keywords: Slurry stability, Digital light printing, Ceramic slurries, 3D printing, Hydroxyapatite slurries.

Effect of Alumina in Reduction of the Iron Ore Fines

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Abstract

The conventional Blast Furnace (BF) route for iron production is highly energy-intensive and contributes significantly to carbon dioxide (CO_2) emissions in the steel industry. With increasing global emphasis on decarbonization and sustainable metallurgy, there is a growing need to understand the reduction behavior of low-grade iron ores, particularly those containing higher levels of gangue such as alumina (Al_2O_3). Alumina is commonly present in many iron ore deposits and is known to influence phase transformation, pore structure evolution, and overall reaction kinetics during reduction. In the present study, the effect of alumina concentration on the hydrogen reduction kinetics of hematite ore was investigated using a vertical tubular furnace under isothermal conditions. Reduction experiments were carried out in a controlled hydrogen atmosphere, and the progress of reaction was monitored through continuous weight-loss measurements. The degree of reduction was calculated as a function of time, and kinetic parameters such as the apparent rate constant and activation energy were determined using suitable reaction models. The results indicate that alumina concentration plays a significant role in controlling the reduction behavior of hematite. At lower alumina levels, reduction proceeds relatively faster with better pore development, facilitating gas diffusion through the product layer. However, as alumina content increases, the overall reduction rate decreases. Higher alumina concentrations promote the formation of denser product layers and alumino-ferrite phases, which reduce pore connectivity and increase diffusion resistance during the sequential transformation from Fe_2O_3 to Fe_3O_4 to FeO and finally to metallic Fe. This results in higher activation energy and lower effective rate constants for high-alumina samples.

Therefore, controlling alumina content in hematite ore is crucial for improving reduction efficiency under hydrogen-based conditions. This study provides a clear understanding of how alumina affects reduction kinetics in a vertical tubular furnace system and offers valuable insights for optimizing ore quality and process parameters in sustainable ironmaking technologies.

Keywords: High alumina Iron ore, alumino-ferrite phases, alumina concentration, reduction kinetics, process optimization.

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Modelling the effect of powder reuse on meltpool dynamics and defect formation in additively manufactured components

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Abstract

The reuse of metal powder in additive manufacturing (AM) provides economic and environmental advantages through reduced raw material consumption and minimised waste. However, powder reuse introduces variability in material properties, impacting part quality and process stability. This study develops a (two-dimensional) 2D numerical model to simulate the additive manufacturing process using a blend of virgin and reused SS316 metal powders. Reused particles incorporate oxidation and composite properties, with oxidation levels determined by the number of reuse cycles. Simulation results reveal that higher fractions of reused powder lead to reduced effective thermal conductivity, destabilisation of the melt pool, and increased susceptibility to defects such as porosity and micro-cracking. The presence of metal-oxide layers on particle surfaces induces viscous drag, impeding fluid flow and promoting the formation of vortices that trap inter-particle gases during melting. These oxide films create discrete regions within the melt pool with distinct thermal and fluid dynamic behaviour, resulting in non-uniform flow patterns and increased microstructural variability. Micro-pore analysis indicates pores below 5 μm are primarily attributed to gas entrapment driven by fluid flow within the mushy zone during the meting process. A proposed strategy seeks to limit oxidation in recycled powders to below 25% by volume, thereby improving cost efficiency while preserving build quality.

Keywords: Additive manufacturing, powder reuse, porosity, defect modeling, numerical model.

Oral Session III A:
Biomaterials and Bioengineering

Agar-based Electrospun Bilayer Dressing for Chronic Wound Management

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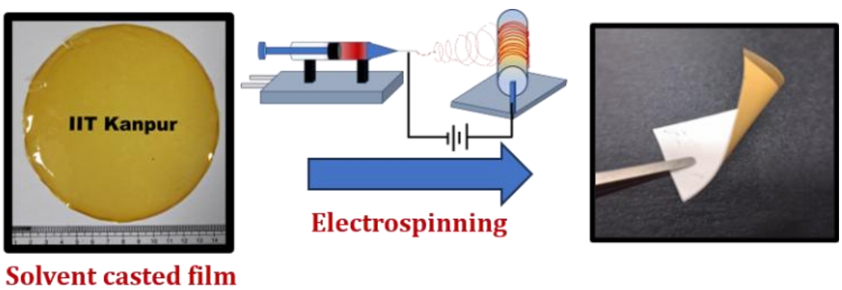
Abstract

Effective chronic wound care requires dressings that combine antibacterial, antioxidant, biocompatible, biodegradable, and fluid-handling properties without compromising any key function. However, no single advanced dressing has demonstrated comprehensive multifunctionality, often compromising one or more critical features essential for effective healing. In this work, agar-based bilayer dressing incorporated with antibacterial and antioxidant agents was developed. The support layer was developed by solvent casting agar, and the primary layer was electrospun over it. The supporting agar base layer containing antibacterial agents was designed for the sustained release of silver nanoparticles, ensuring long-term antibacterial efficacy. The primary electrospun layer demonstrated 98% porosity and was infused with gallic acid, which resulted in a 90% free radical scavenging efficacy. In the interim, the bilayer morphology demonstrated exceptional fluid handling properties, such as an optimal wettability of 64° for cell adhesion and proliferation, an excellent moisture transmission rate of 1200 g/m^2/day, and an enhanced swelling ability of approximately ~250%, which created a moist microenvironment without macerating the wound site. As determined by the time-kill assay, the dressing demonstrated a substantial bacteriostatic effect against both gram-positive and gram-negative microorganisms. High hemocompatibility (98%) and cytocompatibility (>80%) were confirmed by the biocompatibility evaluation. Wound scratch assay demonstrated a wound closure area of over 79%, which confirmed its efficacy for wound care applications. Furthermore, the bilayer dressing's efficacy was evidenced by *in vivo* models, which demonstrated a higher rate of epithelial formation and over 97% healing within 12 days. Overall, this bilayer dressing offers a promising, multifunctional approach for chronic wound management, integrating broad-spectrum antibacterial and antioxidant protection with optimal fluid handling and biocompatibility.

Keywords: Agar, electrospinning, wound healing, nanofibrous, asymmetric dressing.



Asymmetric bilayer morphology comprising an agar-based nanofibrous layer electrospun onto an agar solvent cast base layer, both incorporated with multifunctional agents for enhanced wound healing.

Biological Evaluation of PHD2 Inducers as Potential Anticancer Agents

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Abstract

Hypoxia and abnormal metabolism is the classical feature of cancer. Hypoxia inducible factor (HIF) is a transcription factor and is responsible for the expression of genes that facilitate adaptation and survival of cancer cell in poorly oxygenated condition. HIF is also associated with dysregulated metabolism in cancer. The HIF activity is regulated by oxygen dependent prolyl hydroxylases domain enzyme (PHDs). The aim of present study was to inquest the chemical activation of prolyl hydroxylase-2 for the curtailment of over expressed hypoxia inducible factor-1α and fatty acid synthase (FASN) in mammary gland carcinomas. After screening a battery of compounds, BBAP-1 and BBAP-2 were retrieved as potential prolyl hydroxylase-2 activators and validates their activity using ER+MCF-7 cell line and n-methyl-n-nitrosourea induced rat mammary gland model. BBAP-1 and BBAP-2 shows the morphological characteristics of apoptosis as well as decrease in the mitochondrial permeability as visualized by acridine orange/ethidium bromide and JC-1 staining against ER+MCF-7 cells. Afterward, *in-vivo* studies were scrutinized against n-methyl-n-nitrosourea induced carcinogenesis in albino wistar rats. Both the compounds restored the morphological architecture when screened through carmine staining, hematoxyline and eosin staining and scanning electron microscopy. Both BBAP-1 and BBAP-2 restored oxidative stress markers favourably and also up regulated the Caspase 3 and Caspase 8 levels. The immunoblotting and mRNA expression analysis validated BBAP-1 and BBAP-2 as potential prolyl hydroxylase-2 activator by sequential downregulating effect on hypoxia inducible factor-1α and other downstream targets. BBAP-1 and BBAP-2 produced apoptosis through mitochondria-mediated death pathway. It was concluded that the chemical activation of prolyl hydroxylase-2 can have the potential role in curtailing the growth of tumor cells by down-regulating the expression of HIF-1α and FASN.

Keywords: Hypoxia, Prolyl hydroxylases, Hypoxia-inducible factors , BBAP-1 and BBAP-2.

Effect of Feedstock Characteristics on Cell Adhesion, Mineralization, and Nanomechanical Properties of Suspension Plasma-Sprayed Hydroxyapatite/Bioglass Coatings

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Abstract

The clinical longevity of Ti6Al4V load-bearing implants is compromised by their intrinsic bio-inertness and the mismatch between the stiffness of the alloy (~114 GPa) and the surrounding cortical bone (~15–30 GPa), leading to fibrous encapsulation and stress shielding. The present study addresses these challenges via the development of axial suspension plasma-sprayed (SPS) porous coatings of hydroxyapatite (HA) and 45S5 bioglass (BG). Conventional atmospheric plasma spraying (APS), which is limited to coarse micro-scale powders feedstocks, SPS enables the deposition of nanometre-sized feedstocks to produce thinner coatings (<50 μm). In this study, a micro-sized HA coating deposited by APS (μHA-APS; feedstock particle size 30-40 μm) was used as a reference, while three coatings were fabricated by SPS: micrometre-sized HA (μHA-SPS; 4-5 μm), nanometre-sized HA (nHA-SPS, 300-600 nm), and a nano-sized HA/BG composite (nHABG-SPS; 80% HA–20% BG; 300-600 nm). The μHA-SPS and nHA-SPS coatings enabled evaluation of particle size effects, whereas compositional influences of nHA-SPS and nHABG-SPS were contrasted, where nHA-SPS coating exhibited the highest porosity of ~21% among all other coatings. It is envisaged that the addition of BG (nHABG-SPS) reduced the porosity by 6.5% via pore filling due to its low softening temperature and glassy nature. Higher contact angles (CAs) of nHA-SPS (~129°) and nHABG-SPS (~131%) relative to micro-powder-based μHA-APS and μHA-SPS coatings, indicating that wettability is governed by the combined effects of porosity-induced air entrapment and surface chemistry, with lower surface energy of BG further enhancing hydrophobicity. Subsequently, nHABG-SPS coating exhibited superior cell proliferation (~40% increase), enhanced cell adhesion (~136% higher cell count), and longer filopodial extensions (~40 μm), with aspect ratio of 3.1 indicating an enhanced cell material interaction (cell deposited matrix like deposition), attributed to the protein dominated adhesion (CA>90°) as compared to μHA-SPS. Subsequently, nHA-SPS exhibited the highest mineralization, increased by ~100 % and ~160 % as compared to μHA-APS and μHA-SPS, respectively. Further, nHA-SPS and nHABG-SPS coatings showed reduced nano-hardness (~3.3 and 3.4 GPa, respectively) and Young's modulus (43 and 51.9 GPa, respectively) than micro-particle coatings due to higher porosity and weaker inter-splat bonding, while the addition of BG reduced the elastic modulus without affecting hardness due to its compliant amorphous phase. As a result, this study establishes suspension plasma spraying as a potential surface engineering strategy for tailoring implant coatings that simultaneously enhance bioactivity and achieve bone-like mechanical behavior, thereby improving the long-term performance and clinical reliability of Ti6Al4V load-bearing biomedical implants.

Keywords: Suspension Plasma Spraying, Hydroxyapatite, Cell Adhesion, Biomineralization, Nanomechanical properties.

Bi_2S_3 Electrocatalyst for Non-Enzymatic Electrochemical Glucose Detection: Mechanistic Insights and Sensing in Human Blood and Serum

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Abstract

Non-enzymatic electrochemical glucose sensors based on metal chalcogenides have recently attracted considerable attention due to their high catalytic activity and structural tunability. In this work, we investigate the electrocatalytic behavior of Bi_2S_3 toward glucose oxidation. Bi_2S_3 nanostructures were synthesized via a facile hydrothermal route. A binder-free, two-step hydrothermal electrode fabrication strategy enabled the formation of a high-surface-area electrode with abundant redox-active sites for efficient glucose interaction. Detailed structural and morphological characterizations confirmed the orthorhombic crystal structure and porous nature of the synthesized Bi_2S_3. Electrochemical investigations demonstrate that the Bi2S3-modified electrode exhibits exceptional electrocatalytic activity for glucose oxidation in alkaline media. The developed sensor achieves high sensitivity, a low limit of detection (LOD), and a wide linear detection range. To elucidate the sensing mechanism, Density Functional Theory (DFT) calculations were employed to analyze electronic interactions between glucose and the catalyst surface, thereby identifying the primary charge-transfer pathways and the active nucleophilic sites. Furthermore, the practical applicability of the sensor was validated through glucose detection in complex biological matrices, including human blood and serum samples, demonstrating excellent recovery and minimal interference from common endogenous species. These results highlight Bi_2S_3 as a promising and cost-effective platform for next-generation enzyme-free glucose sensing and point-of-care diagnostics.

Keywords: Biosensor; Detection limit; Sensitivity; Glucose oxidation; Binder free electrode.

Oral Session III B:

Modelling and Simulation in Materials Science and Engineering

A Hybrid Phase-Field and Deep Learning Framework for Predicting 2D and 3D Microstructure Evolution in Ternary Alloys

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Abstract

We develop a hybrid framework that integrates phase-field modelling (PFM) with an attention-enhanced deep learning (DL) architecture to enable accurate and computationally efficient prediction of microstructure evolution. Phase-field simulations provide the physically consistent description of microstructure evolution and generate high-fidelity datasets, while the DL architecture learns complex spatiotemporal patterns and extends predictions to longer times and larger systems. To demonstrate the capability of this approach, we investigate complex ternary alloy systems and capture three distinct phase-separation mechanisms that arise during the early stages of spinodal decomposition in both two and three dimensions. The DL methodology incorporates three key components: a dimensionality-reducing autoencoder for efficient representation of high-resolution microstructure images (256×256×3), an attention-augmented Convolutional Long Short-Term Memory (ConvLSTM) network for learning complex spatiotemporal evolution patterns, and a slice-by-slice strategy for predicting three-dimensional systems (128×128×128×3). Within this framework, PFM resolves the rapid early-stage evolution of microstructures, while the trained DL model predicts the subsequent coarsening behaviour with significantly reduced computational cost. The DL model demonstrates strong predictive capability, accurately forecasting microstructure evolution up to 400 timesteps ahead, including for compositions outside the training set. By combining the predictive efficiency of deep learning with the physical fidelity of phase-field modelling, this framework establishes a powerful platform for studying complex multicomponent microstructure evolution.

Keywords: Phase-field Model, Spinodal Decomposition, Ternary Alloy, Deep Learning, GPU acceleration.

Crystallization and Heat Transfer Behaviour of Mould Fluxes in Continuous Casting of Peritectic Steel

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Abstract

Optimizing the properties of mould flux is essential for managing heat transfer and lubrication during the continuous casting of peritectic steels, as inadequate thermal control can result in transverse cracking and surface imperfections. This research explores the optimization of mould powders for casting JA69BMQT-05 peritectic steel slabs by integrating compositional analysis, thermophysical modeling, and experimental characterization. Industrial mould fluxes (667P and 816BS) were assessed alongside laboratory-designed flux compositions (F1 and F2) to examine their crystallization behavior and impact on heat transfer. Thermophysical properties, including glass transition temperature, liquidus temperature, viscosity, and crystallization tendency, were estimated using established empirical models and validated through differential scanning calorimetry (DSC). The crystalline fractions of the slags were quantified using Li-test prepared samples, followed by SEM-EDS phase identification and ImageJ-based area fraction analysis. The experimental findings revealed crystalline fractions of about 60.1% for 816BS and 61% for 667P, with cuspidine identified as the primary crystalline phase influencing heat transfer in the mould flux film. Further XRD analysis showed higher crystallinity in the laboratory-designed flux F1 (≈80%) compared to F2 (≈54%). A heat-transfer model incorporating slag film structure, viscosity, and crystallization fraction was developed to estimate heat flux, slag film thickness, and shell growth during casting. Model predictions suggested that the F1 composition offers the lowest meniscus heat flux and the thickest liquid slag layer, leading to enhanced lubrication and reduced thermal stress compared to industrial fluxes. The findings indicate that designing mould flux with controlled basicity, moderate crystallization, and optimized viscosity can significantly enhance thermal regulation and lubrication during casting. The proposed methodology, which combines compositional screening, thermal analysis, microstructural characterization, and heat-transfer modeling, provides a comprehensive framework for designing mould fluxes tailored for peritectic steel casting applications.

Keywords: Continuous Casting; Mould Flux Optimization; Peritectic Steel; Crystallization Behaviour; Heat Transfer in Mould Flux; Differential Scanning Calorimetry (DSC).

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Research Scholars' Day on Metallurgy and Materials

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Effect of Ti Addition on Screw-Dislocation Mediated Plasticity in W-Containing Refractory High-Entropy Alloys

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Abstract

Refractory high-entropy alloys (RHEAs) based on group-V and group-VI transition metals are promising candidates for extreme-environment applications, including plasma-facing components in fusion reactors, owing to their high melting temperatures and radiation tolerance. However, the practical use of tungsten-containing RHEAs with a body-centered cubic (BCC) crystal structure is severely limited by their intrinsic brittleness at room and relatively low temperatures. Consequently, improving the ductility of BCC RHEAs remains a critical challenge. Plastic deformation in BCC metals and alloys is primarily governed by the mobility of ½<111> screw dislocations, which therefore play a decisive role in determining their plasticity. In this work, we investigate the effect of a minor Ti addition (5 at.%) on the intrinsic ductility of the W-containing RHEA, $W_{0.36}Ta_{0.36}Nb_{0.28}$, using density functional theory (DFT) in conjunction with experimental techniques. DFT calculations show that Ti addition promotes a non-compact dislocation core configuration and reduces the Peierls barrier, thereby facilitating screw-dislocation motion. Consistent with these predictions, experimental results reveal enhanced plastic strain and increased screw-dislocation mobility. Dislocation structures were further characterized using controlled electron channeling contrast imaging (cECCI). Long, straight screw dislocations were observed in $W_{0.36}Ta_{0.36}Nb_{0.28}$, whereas cusped dislocations were identified in $(W_{0.36}Ta_{0.36}Nb_{0.28})Ti_{0.05}$. The Ti addition promotes the formation of superjogs, which act as temporary pinning points and contribute to simultaneous improvement in strength and ductility. This behavior closely resembles the ductilizing effect reported in W–Re alloys. Slip-trace analysis further reveals that deformation in the base RHEA is dominated by {110} slip, while Ti addition activates {112} slip systems and promotes frequent cross-slip. These findings establish the operative deformation mechanisms responsible for the improved ductility in Ti-modified W-containing RHEAs.

Keywords: Refractory high-entropy alloy (RHEA); Density functional theory (DFT); Screw Dislocations; electron channeling contrast imaging (ECCI).

Effect of Magnetic Field on Grain Growth in Polycrystalline Materials: A Phase Field Study

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Abstract

In this study, we employ a phase-field model to investigate how an external magnetic field influ-ences grain growth in diamagnetic materials, with a particular focus on bismuth. Grain growth in strain-free materials is primarily driven by grain boundary curvature, which acts to minimize the overall interfacial energy. However, in materials with anisotropic magnetic susceptibility, such as bismuth, an applied magnetic field introduces an additional driving force that can modify grain growth behavior. Simulations were performed for both bicrystal configurations and large polycrystalline systems comprising 1000 grains with randomly distributed orientations. The results demonstrate that the application of magnetic fields significantly accelerates grain growth relative to the zero-field case. Kinetic analysis based on the temporal evolution of the average grain diameter squared, ⟨d⟩2, exhibits a linear trend, confirming normal grain growth kinetics. Moreover, the slope of ⟨d⟩2 versus time systematically increases with magnetic field strength, indicating an enhancement in the effective grain growth rate. Overall, the study establishes that the proposed phase-field model accurately captures the coupled curvature-driven and field-driven contributions to grain growth. These findings provide a mechanistic understanding of magnetically assisted microstructural evolution and highlight the potential of external fields for tailoring grain growth and texture development in diamagnetic polycrystals.

Keywords: Grain growth, Phase field modelling, Magnetic field, Polycrystalline metals.

Poster Presentations :

Sustainable Recovery of Metals and Polymers from End-of-life Photovoltaic modules & Waste Printed Circuit Boards

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Abstract

The increasing amount of solar photovoltaic (PV) panels and waste printed circuit boards (WPCBs) has become a serious environmental problem today. Both types of waste contain valuable metals like copper, silver, nickel, aluminium and important polymers like EVA and epoxy resin. Therefore, they should be considered useful resources for recycling rather than being thrown away. But a review of the literature shows that most research considers the recycling of solar panels and WPCBs as separate processes. This causes recycling processes to be complex, require more chemicals and energy, and go through multiple steps. As a result, problems such as incomplete delamination, low metal selectivity, and limited polymer recovery are often encountered. To overcome these limitations, the presented work proposes an Integrated Recycling approach, in which both solar panels and WPCBs are treated in the same framework. Instead of separate processes, this approach allows for selective metal recovery and effective polymer separation using the same conditions, reducing chemical use and environmental impact. By combining metals and polymer recovery into a combined route, this approach simplifies the overall process, reduces waste, and promotes the circular economy. The aim of this study to provide an overview of literature pertaining the recycling of WPCBs and solar panel to develop methods for combined recycling.

Keywords: Sustainable recovery, WPCB, Solar panel, circular economy.

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Mechanistic insights into hydrogen-metal interactions in aerospace-grade advanced high-strength titanium alloys

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Abstract

The interaction of hydrogen with metallic materials has been widely studied due to its detrimental influence on their mechanical properties. Hydrogen embrittlement (HE) is a major concern in structural materials such as steel, aluminum, zirconium, and titanium alloys, often leading to premature failure during service. Several mechanisms have been proposed to explain hydrogen embrittlement, including hydrogen-enhanced localized plasticity (HELP), hydrogen-enhanced decohesion (HEDE), and absorption-induced dislocation emission (AIDE). These mechanisms may act individually or together, depending on the material and environmental conditions. However, understanding the interaction of hydrogen with materials at the atomic scale remains challenging because of its small size and high diffusivity.

Titanium alloys are widely used in aerospace and industrial applications because of their high strength-to-weight ratio and corrosion resistance. Among them, α+β alloys such as Ti-6Al-2Sn-4Zr-6Mo and metastable β alloys like Ti-5Al-5Mo-5V-3Cr are commonly used in critical structural components. Under demanding service conditions, hydrogen ingress can significantly affect their deformation behavior and structural integrity.

This study presents an overview of hydrogen–metal interactions and the mechanisms responsible for hydrogen embrittlement in advanced titanium alloys. The focus is on understanding factors controlling hydrogen uptake and their influence on mechanical behavior, highlighting the need for further research in this area.

Keywords: Hydrogen embrittlement; Titanium alloys; Hydrogen–metal interaction; HELP; HEDE.

ZrB_2 based Functionally Graded Ultra High Temperature Ceramics (UHTCs) for Hypersonic Vehicles

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Abstract

Hypersonic vehicles experience extreme aerodynamic heating, particularly at their leading edges, where temperatures can exceed 2000°C due to intense friction and shock wave interactions. Traditional materials fail under such extreme thermal and mechanical conditions, necessitating the use of Ultra-High Temperature Ceramics (UHTCs)—a class of refractory materials with melting points exceeding 3000°C, exceptional oxidation resistance above 1500°C, and high thermal conductivity (~40–60 W/m·K). Over the past few decades, extensive research has focused on transition metal borides (ZrB_2, HfB_2), carbides (ZrC, HfC), and nitrides (HfN, ZrN) due to their high melting points (ZrB_2: ~3246°C, HfC: ~3890°C, HfN: ~3305°C), oxidation resistance in excess of 1800°C, and moderate thermal expansion coefficients ($\sim 6\times10^{-6}$ K^{-1}). However, despite these promising properties, UHTCs face inherent challenges such as intrinsic brittleness (fracture toughness ~3–4 $MPa\cdot m^{1/2}$), poor thermal shock resistance, and limited damage tolerance, which restrict their practical application in aerospace environments. Current thermal protection system (TPS) architectures based on monolithic UHTCs or discrete ceramic coatings exhibit abrupt mismatches in thermophysical and mechanical properties between the substrate (typically C/C or SiC-based composites) and the protective layer. Coefficients of thermal expansion can differ from $\sim 3\text{–}4\times10^{-6}$ K^{-1} (C/C) to $\sim 6\text{–}7\times10^{-6}$ K^{-1} (ZrB_2–HfB_2 UHTCs), generating residual thermal stresses exceeding 300–600 MPa during heating–cooling cycles with temperature gradients of 1000–2000 °C. Such stress concentrations promote interfacial delamination, coating spallation, and microcrack formation, particularly under repeated hypersonic flight cycles ($>10^2\text{–}10^3$ thermal cycles). Functionally graded materials (FGMs) provide an effective pathway to mitigate these limitations by enabling a continuous or stepwise gradient in composition and microstructure across thicknesses typically ranging from 100 µm to several millimeters. By gradually varying UHTC content from ~10–20 vol.% at the substrate interface to >80–90 vol.% at the surface, FGMs can reduce interfacial thermal stresses by 30–60%, while improving thermal shock resistance by a factor of 1.5–2 compared to monolithic coatings. Tailored gradients in thermal conductivity ($\sim 10\rightarrow 50$ $W\cdot m^{-1}\cdot K^{-1}$) and elastic modulus (~100→500 GPa) help distribute heat fluxes exceeding 1–5 $MW\cdot m^{-2}$ more uniformly, minimizing localized damage. In this context, functionally graded UHTCs emerge as a transformative TPS strategy, combining surface-level temperature capability beyond 2000–2500 °C with enhanced fracture resistance, interfacial adhesion strength (> 30–50 MPa), and improved damage tolerance under hypersonic thermo-mechanical loading. This study provides an understanding of the processing strategy and microstructural evolution in functionally graded UHTC materials. Hardness profiling together with SEM and BSE imaging is employed to examine the gradient architecture and assess the mechanical and microstructural characteristics of the fabricated FG system.

Keywords: Ultra High Temperature Ceramics (UHTCs), Hypersonic Vehicles, Functionally Graded Material (FGM), Thermal Protection System (TPS).

Microstructural and Mechanical characterization of Additively Manufactured Stainless Steel - Mild Steel Functionally Graded Material (FGM) for pipeline application

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Abstract

This work demonstrates functionally graded material (FGM) fabrication via wire arc additive manufacturing (WAAM) as a novel solution for minimizing the brittleness and cracking between mild steel and stainless steel (MS-SS). A FGM consisting of three-zones with different compositions were deposited: top-zone of stainless steel (3 mm thick), intermediate zone of 50% MS - 50% SS (3 mm thick), and bottom zone composed of MS with a 7 mm thick baseplate. This FGM was fabricated utilizing a precision wire feedstock with switching controlled the gradient composition.

Microstructural analysis of the functionally graded material (FGM) was carried out using OM, SEM, EDS, and EBSD. The 100% stainless steel (SS) zone exhibited a dendritic microstructure, enriched in Fe, with chromium-rich $M_{23}C_6$ carbides in the inter-dendritic regions and minor δ-ferrite within the austenitic matrix. In contrast, the 50% mild steel - 50% SS zone showed a mixed microstructure dominated by bainite and martensite. No interfacial cracks or delamination were observed, indicating excellent metallurgical bonding. EBSD revealed randomly oriented columnar grains in the 100% SS zone, while the mixed zone featured fine, needle-like grains due to the presence of complex phase mixtures. Vickers microhardness testing revealed hardness values of 175 HV, 380 HV, and 133 HV for the 100% SS, 50% MS–50% SS, and MS plate regions, respectively. The elevated hardness in the intermediate zone is attributed to the formation of hard phases such as bainite and martensite. XRD analysis further confirmed the phase constituents across the graded layers.

Keywords: FGM, WAAM, interfacial bonding, Stainless Steel, Mild Steel.

Perovskite TE-Predictor: An Interpretable Machine Learning Framework to Accelerate the Design of Oxide-Perovskite Thermoelectric Materials

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Abstarct

A thermoelectric (TE) power generator converts waste heat from manufacturing industries, power plants, and combustion engines into electricity, providing a sustainable energy solution. Oxide perovskites (ABO_3) are promising TE materials due to their thermal stability and environmentally benign nature, but their low figure-of-merit (zT) limits energy conversion efficiency. Designing high-zT oxide perovskites is crucial for making it a viable option for practical applications. In this study, machine learning (ML) is employed to predict TE properties of ABO_3. A dataset of 110 perovskite compositions has been curated from literature, including experimental data on the Seebeck coefficient, electrical conductivity, thermal conductivity, and zT at various temperatures. Elemental and structural properties are used for featurization, with the positional-average elemental property (PAEP) approach to capture site-specific effects and improve model accuracy. Ensemble learning models, specifically bagging and boosting algorithms, are utilized and have achieved high predictive accuracy with R2 >0.90. SHAP is utilized to explain the trained models, to show these models are not just highly accurate but also able to capture the science behind the predictions. Finally, a GUI-based Perovskite TE-Predictor is developed to integrate these models for real-time, temperature-dependent predictions of any oxide perovskite composition. To the best of our knowledge, this is the first ML-based study to predict zT for oxide perovskites, highlighting ML's potential to accelerate the discovery of high-performance TE materials.

Keywords: Thermoelectric, Machine Learning, Perovskites.

Structural Engineering of Doped P2-Type Layered Oxides for High-Stability Sodium-Ion

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Abstract

With the growing need for large-scale energy storage, electrochemical energy storage offers a promising solution due to its high energy density and efficiency. Although lithium-ion batteries are widely used in portable electronics and electric vehicles, their large-scale deployment for grid storage is restricted by the limited availability and high cost of lithium resources. Sodium-ion batteries (SIBs) are emerging as an alternative, with layered transition-metal oxides, typically P2-type Na_xMnO_2 (x = 0.6-0.8), drawing significant interest for their high theoretical capacity (~170 mAh g^{-1}) and high-voltage stability (~4V). However, these materials typically exhibit irreversible phase transitions at high voltages, substantial structural distortions, and poor air stability, resulting in low cycle life and poor rate capability and collectively limiting their commercialization.

The current study investigates the strategic modification of P2-type layered oxides via multi-element aliovalent cation doping at transition-metal sites. Utilizing the Pechini sol-gel method for precise composition and morphology control, this research explores the integration of cations of different ionic radii into the host lattice to tune the interlayer spacing. The introduction of aliovalent dopants serves to stabilize the crystal framework, effectively suppressing the irreversible phase transitions and Jahn-Teller-induced distortions common in manganese-rich systems. By engineering the local chemical environment, this approach aims to achieve a significant increase in capacity retention and structural robustness over extended cycling. The results emphasize the correlation between dopant-induced lattice expansion and electrochemical performance, providing a pathway toward high-performance cathode materials for next-generation sodium-ion storage.

Keywords: Layered oxides, Jahn- Teller Distortion, Structural Engineering, Aliovalent Doping, Cycling Stability.

High-Entropy Design Strategy for Ultralow Thermal Conductivity in p-Type Oxide Thermoelectric

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Abstract

Recent studies in high-entropy oxides have demonstrated their potential as next-generation functional materials for high-temperature thermoelectric (TE) applications. Their atomic-level disorder provides a higher-order phonon scattering to suppress thermal conductivity while maintaining structural stability, which has been difficult to achieve in conventional oxides due to their inherently short phonon mean free paths. However, n-type TE oxides are widely studied, and p-type TE oxides remain less explored. In this study, we report the synthesis of a novel high-entropy p-type perovskite oxide, $Sr(Cr_{0.2}Mn_{0.2}Fe_{0.2}Sn_{0.2}Co_{0.2})O_3$, synthesized by the conventional solid-state reaction route. X-ray diffraction confirms the phase purity of the perovskite structure, and scanning electron micrograph with elemental mapping (EDXS) demonstrates a dense microstructure. The multi-cation substitution at the B-site in $Sr(Cr_{0.2}Mn_{0.2}Fe_{0.2}Sn_{0.2}Co_{0.2})O_3$ effectively suppresses phonon transport with an ultralow thermal conductivity of 0.94 W/mK at 325 K, which remains consistently close to ~1 W/mK across the temperature range (300 - 1100 K). Thermally activated carrier transport enhances electrical conductivity to ~400 S/m at 1056 K, leading to a maximum figure of merit (zT) of 1.2×10^{-4} at 1056 K. This study shows the potential of high-entropy design in achieving ultralow thermal conductivity in p-type oxide systems at elevated temperatures.

Keywords: High-Entropy Design**,** p-type oxide, electrical conductivity.

Effect of Solutionizing Duration on Microstructure and Fretting Tribocorrosion Behavior of AZ91

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Abstract

Magnesium alloys such as AZ91 are excellent candidates for lightweight structural and biomedical applications; however, their meager tribo-corrosion resistance limits their wider implementation. The present study investigates the influence of solutionizing duration on the microstructural evolution and tribo-corrosion behavior of AZ91 magnesium alloy. Samples were solution treated at 420 °C under vacuum-sealed quartz tube conditions for varying durations (0.25, 0.5, 1, 2, 5, and 24 h), followed by water quenching. Microstructural characterization was performed using scanning electron microscopy (SEM) to evaluate the dissolution behavior of the β-$Mg_{17}Al_{12}$ phase.

Results indicate progressive dissolution and fragmentation of the β-phase network with increasing solutionizing time, leading to a more homogenized α-Mg matrix. Short treatment durations retained semi-continuous β networks, promoting micro-galvanic coupling, whereas longer durations significantly reduced β-phase continuity.

The modified microstructure directly influences the tribocorrosion response by altering the balance between mechanical wear and electrochemical degradation. Reduction of continuous β-phase networks is expected to mitigate localized galvanic corrosion under fretting conditions. The study highlights the importance of optimizing solutionizing time to balance phase dissolution and microstructural stability for improved degradation resistance of AZ91 alloy under fretting conditions.

Keywords: Solutionizing, Micro-galvanic corrosion, Fretting tribocorrosion, AZ91 magnesium alloy.

Subgrain detection in ebsd dataset using clustering ML models

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Abstract

Sub-grains, which arise from the rearrangement of geometrically necessary dislocations (GNDs), are essential for accommodating lattice curvature and maintaining strain compatibility during plastic deformation. Their distribution and orientation greatly affect the overall texture evolution of polycrystalline materials, thereby influencing mechanical properties such as strength and anisotropy. Nonetheless, identifying sub-grain boundaries is a significant challenge due to their naturally low misorientation angles (<15°). Conventional segmentation methods that rely on fixed misorientation thresholds often incorrectly classify noise as structure or overlook subtle orientation gradients. In this study, we introduce a computational pipeline utilising the Orix Python library to analyse EBSD data from deformed Cu samples. The methodology encompasses pixel-wise orientation extraction, misorientation calculations with nearest neighbours, and visualisation of dislocation-induced substructures. We implement and compare two advanced models for sub-grain detection: Fast Multiscale Clustering (FMC), which identifies orientation clusters with varying sensitivity levels, and Anti-Leak Grain Identification (ALGrID), which reconstructs closed boundaries using a graph-based approach centred on disorientation paths. While FMC successfully reveals gradual transitions, ALGrID is more effective at minimising false segmentation and capturing connected structures. This integrated framework improves the accuracy and automation of sub-grain segmentation, facilitating quantitative analysis of GND-driven microstructural evolution and texture development.

Keywords: Subgrain detection, microstructural evolution, texture development.

Creep life prediction of P91 grade steel using Genetic Algorithms and Physics-Informed Neural Network

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Abstract

This study is focused on understanding and predicting the complex creep behaviour in P91 grade steels, a critical material extensively utilised in high-temperature industrial applications such as advanced power generation plants. The methodology consists of discovering the underlying mathematical relationship between operating temperature, applied stress, chemical composition, microstructural properties, and equilibrium phase fractions calculated from CALPHAD (Calculation of Phase Diagram) using ThermoCalc. It is well established that creep-rupture life exhibits highly non-linear behaviour in different materials under varying conditions of temperature and stress, complicating long-term structural integrity assessments. Historically, the creep equations that have been discovered and utilised are largely based on empirical results derived from extensive experimental observations, which often struggle to extrapolate accurately beyond their specific tested ranges. In recent times, a lot of successful attempts have been made to derive a mathematical relationship between creep rupture life, experimental conditions, and material chemistry, especially with the help of advanced machine learning techniques. However, many conventional data-driven models act as "black boxes," capturing statistical correlations without offering meaningful insights into the underlying metallurgical or physical degradation mechanisms. To address this limitation, we have employed Multi-Gene Genetic Programming (MGGP) coupled with symbolic regression to discover a transparent mathematical equation that accurately explains creep behaviour in our chosen material of interest. MGGP is inspired by the principles of natural evolution and biological genetics, simulating processes like crossover and mutation to evolve multigene families into optimal mathematical expressions. The obtained best-fitting equation is predominantly a function of temperature and stress, exhibiting a lesser dependency on variations in material chemistry and phase ratios. Crucially, this derived equation is directly integrated into a Physics-Informed Neural Network (PINN) to serve as the governing underlying physical basis for the model. By embedding this explicit mathematical relationship into the network, the hybrid MGGP-PINN approach effectively constrains the learning process to obey known physical boundaries. This novel methodology demonstrates excellent predictive capabilities for creep rupture life on unseen test data.

Keywords Creep, Machine Learning, Multi-Gene Genetic Programming, Creep-rupture, P91 steel.

Physics-Informed Machine Learning Framework for Magnetic High-Entropy Alloys with Experimental Validation

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Abstract

High-Entropy Alloys (HEAs) offer a versatile compositional platform for tailoring magnetic properties for advanced soft magnetic applications. This work presents an integrated computational–experimental framework combining thermodynamic screening, structured data engineering, and physics-informed machine learning for predicting saturation magnetization (M_s) and coercivity (H_c). A curated literature database comprising alloy compositions, synthesis routes, thermodynamic descriptors, microstructural parameters, and magnetic measurements was constructed. Alongside elemental fractions, physics-informed features including valence electron concentration (VEC), average magnetic moment (Zm_{avg}), and atomic size mismatch () were incorporated to enhance predictive interpretability. To ensure statistically balanced learning across the magnetization spectrum, the dataset was stratified into low, intermediate, and high M_s regimes, and an iterative, non-repetitive region-wise sampling framework was implemented to maintain uniform representation while preventing sample reuse across training cycles. Supervised regression models were developed using XGBoost and evaluated using R2, MAE, RMSE, and slope-based physical consistency analysis from predicted-versus-literature plots. For H_c prediction, uncertainty-aware modeling was explored to address grain-size-dependent variability. Experimental validation on arc-melted FeCoNi-based alloys, characterized using X-ray diffraction and vibrating sample magnetometry (VSM), confirmed the robustness and reliability of the proposed framework.

Keywords: High-Entropy Alloys; Materials Design; Machine Learning; Magnetic Properties.

Development of Cost-Efficient Environmentally Friendly Thermoelectric Material

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Abstract

The growing global energy demand and environmental concerns have intensified the search for sustainable energy solutions. Thermoelectric materials offer a promising pathway by directly converting waste heat into electricity without a carbon footprint and environmental noise. Thermoelectric generators have solid-state design, with no moving parts or chemical reactions, enables compactness, low maintenance, and long-term reliability. The conversion efficiency of a thermoelectric generator is generally expressed by thermoelectric figure of merit (zT); where as $zT = (S^2\sigma)T\kappa^{-1}$, here S stands for Seebeck coefficient, σ represents electrical conductivity, T is absolute temperature and κ depicts thermal conductivity. It is tricky to improve zT as all the components in zT are strongly co-related. Chalcogenide based materials such as Pb base tellurides, selenides are popular candidates for thermoelectric generators owing to their high zT and low electrical band gap. However, inherent environmental hazard, toxicity as well as scarcity of those materials compelled research community to shift their focus to sulfides. Although sulfur's environmentally benign nature and earth abundance are beneficial, low electrical conductivity hurts. Among all the available environmentally benign sulfides, Bismuth sulfide stands out as it shows low thermal conductivity (~0.4 $Wm^{-1}K^{-1}$) and good Seebeck coefficient (~450 μVK^{-1}). However, Bi_2S_3 suffers from low zT (~0.11 at 573-723K) when compared to other Bi based chalcogenides. The low zT is attributed to its higher band gap (~1.5 eV at 298K) as well as higher electrical resistivity. So, to enhance the thermoelectric efficiency of Bi_2S_3, I am developing advanced solid solutions incorporating 2D transition metal chalcogenides (TMDC) viz VS_2. VS_2 is an emerging 2D material with metal like conductivity. VS_2 necessarily improves mechanical strength, electrical conductivity and carrier mobility while suppressing thermal conductivity through enhanced phonon scattering, leading to higher zT values. Integrating such advanced materials into thermoelectric systems holds great potential for sustainable energy.

Keywords: Sustainable energy, Thermoelectric materials, Bismuth sulfide, Vanadium Sulfide.

High entropy oxides as the next generation high temperature thermoelectric material

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Abstract

Recently, entropy-stabilization has been posited as a novel approach for improving the performance of oxide-based thermoelectric materials. The presence of multiple ions increases the configuration entropy of the system, leading to a stable single phase. From the thermoelectric perspective, the entropy stabilization can affect performance by introducing high-order of point defects leading to enhanced phonon scattering, thus reducing the lattice thermal conductivity. Moreover, entropy stabilization provides flexibility of manipulating charge carriers by incorporating higher or lower valence ions to control electrical transport and the entropy stabilization effect can increase the crystal symmetry and thus improve the Seebeck coefficient. Here, we have investigated the influence of the entropy stabilization approach on the thermoelectric performance of the (Ba0.1Ca0.1La0.05Sr0.75)(Ti0.85Nb0.15)O3 ceramics achieved through the isovalent doping of Ba and Ca at the A-site of the La and Nb co-doped $SrTiO_3$ system. A peak zT of 0.28 at 1073 K has been achieved. At last, a thermoelectric module has been fabricated with 4 legs, which has shown the highest power output and power density of 95.5 mW and 2902 W/m^2 for any oxide module ever reported.

Keywords: Thermoelectric, oxide, high entropy, module.

Physics-Informed Neural Network for Stress Analysis in In-Plane Crack Problem

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Abstract

Physics-Informed Neural Networks (PINNs) provide a powerful framework for embedding governing equations of fracture mechanics directly into machine learning models, enabling meshless simulations of crack problems with improved computational efficiency while upholding physical accuracy. Traditional neural networks often struggle to capture the sharp singularities at crack tips, leading to inaccurate stress predictions even with extensive datasets. In this work, we present a PINN-based approach for Mode I crack problems, verified against finite element analysis (FEA). As an initial step, pre-crack analysis of an AA-2050 single-edge notched tension (SENT) specimen is performed in Abaqus, with von Mises stress fields extracted from the first three time steps on a three-dimensional grid. A baseline neural network is trained on these datasets to reproduce global stress trends, forming a benchmark for physics-informed extensions. Building upon this, stress field equations are incorporated into the loss function to create a PINN, enabling stress reconstruction from sparse data while respecting governing physics. Extensions including domain decomposition for improved local resolution and advanced architectures for enhanced efficiency are also explored. This methodology positions PINNs as a promising surrogate modeling tool for fracture mechanics, bridging data-driven and physics-based approaches with potential applications in rapid parameterized testing, failure analysis, and structural integrity assessment of advanced alloys.

Keywords: Physics-Informed Neural Networks, Fracture Mechanics, Finite Element Analysis, Integrated Computational Materials Engineering, AI/ML for Materials Design.

PANI-Derived Microporous Activated Carbon with Ultra-High Surface Area for Efficient Removal of Cationic and Anionic Dyes from Wastewater

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Abstract

Microporous activated carbon was prepared from PANI composite by carbonization at 400 °C followed by chemical activation using KOH at 750 °C. The activated carbon (AC) exhibited a well-developed microporous structure with a high specific surface area (1912.19 m^2/g), average pore radius ≈8.6 Å, and total pore volume 0.8235 cm^3/g as determined by Brunauer-Emmett-Teller method. Field-emission scanning electron microscopy images revealed a rough, highly porous surface. Fourier transform infrared spectroscopic study confirmed the alcoholic and carboxylic hydroxyl groups, confirming abundant surface functional groups (–OH, C=O, –COOH, etc.) to facilitate adsorption. Batch adsorption experiments were conducted on cationic dyes namely methylene blue (MB), Rhodamine B (RhB), crystal violet (CV) and an anionic dye, Congo red (CR). The adsorption reactions were carried out at an initial concentration of 1000 mg/L for MB and 2000 mg/L for RhB, CV and CR (in 20 mL solution) with a fixed optimized adsorbent dosage of 3 g/L, at neutral pH and incubation times up to 24 hours at 150 rpm rotary shaker. The activated carbon obtained from PANI composites exhibits exceptional removal potential for all four dyes. The adsorption kinetics follows the pseudo second order (PSO) model (R^2 = 0.997-0.999), which shows the predominance of chemical adsorption. The equilibrium data follows the Langmuir isotherm model (R^2 = 0.989 to 0.999), which indicated monolayer coverage on a homogeneous surface of AC. The developed activated carbon exhibited high adsorption capacity, with maximum adsorption capacities of 496.85, 816.91, 1035.69, and 1028.03 mg/g for MB, RhB, CV, and CR, respectively, in aqueous medium. Finally, the thermodynamic parameters showed that methylene blue adsorption was an endothermic and spontaneous process; the $\Delta H°$ & $\Delta G°$ values for activated carbon were 52.57 kJ/mol and −105.81 to -111.18 kJ/mol, respectively. These results demonstrate that PANI composite-derived microporous AC is a promising adsorbent for rapid and efficient dye removal from wastewater.

Keywords: Polyaniline (PANI); Chemical activation; Activated carbon (AC); Dye adsorption; Langmuir

Performance Analysis of Thermoelectric Generators for Industrial Applications

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Abstract

Energy requirement in current day is met by utilizing fossil fuels, however, consuming these fossil fuels extensively has become responsible for global warming and climate change. Only one-third of the input energy is used efficiently; the rest gets wasted in the form of heat. Therefore, a device with the ability to generate electricity using waste is highly desirable. Thermoelectric (TE) generators have this fascinating aspect transforming waste thermal energy into electrical energy using the Seebeck effect. Similarly, combustion engines in aircraft and vehicles convert only 20–40% of fuel energy to practical work, with the rest lost as heat. This widespread thermal loss represents a largely untapped energy resource. The study uses in-laboratory developed n-type composite Nb doped and p-type thermoelectric materials exhibiting high figure of merit and high temperature stability, allowing operation in high temperature environments. Numerical modelling and Finite element method (FEM), using COMSOL Multiphysics for a commercial module of 254 legs with a π configuration was performed using isoflux boundary conditions, as well as evaluating performance under different load conditions and contact impedances. Thermoelectric generator (TEG) optimization efforts use parametric sweeping of geometric variables, including leg dimensions, spacing and fill factors, to maximize power generation for our proposed application. Ansys CFX simulations of simplified turbine assemblies provide temperature and heat flux distributions on turbine casings, enabling us to understand realistic boundary conditions for integrated TEG-turbine modelling. Modelling and performance analysis of a commercial TEG module helps us simulate the working of TEGs for our proposed integration conditions. Combining materials characterization and finite element analysis demonstrates significant potential for TEG integration in commercial aviation.

Keywords: Thermoelectric generators, high-temperature applications, turbofan engines, Finite Element Method, thermoelectric materials

Design of Composite Polymer Interface for High-Performance Na-ion Solid-State Batteries

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Abstract

Solid-state sodium-ion batteries (SSSIBs) have emerged as a promising alternative to lithium-ion batteries, offering enhanced safety, thermal stability, and cost-effectiveness. Despite their potential, the practical performance of SSSIBs is often hindered by poor interfacial compatibility between the rigid ceramic solid electrolyte (SE) and the cathode, particularly under ambient conditions and high current operations. To address this limitation, this study introduces a simple and effective strategy involving a composite polymer interface modifier (CPIM) to enhance the cathode–SE interface. The incorporation of CPIM significantly enhances ionic transport and interfacial contact, resulting in stable and efficient electrochemical performance.

The modified half-cell SSSIBs delivered an initial discharge capacity of ~90 mAh/g (theoretical capacity ~109 mAh/g) with minimal degradation, retaining ~82% over extended cycling of 280 cycles at a 1C rate at RT. The modified full-cell SSSIBs, with the same active material loading at the cathode and anode sides, delivered ~45 mAh/g (theoretical capacity ~58.8 mAh/g) at a C/5 rate with 89% capacity retention over 200 cycles at RT.

The improved performance is primarily attributed to the CPIM's high ionic conductivity and its ability to form a more conformal, conductive interface between the cathode and the solid electrolyte. This reduces charge-transfer resistance and promotes efficient sodium-ion movement across the interface.

Overall, this approach highlights the potential of polymer-based interface engineering to overcome key interfacial challenges in SSSIBs, contributing to the development of reliable and sustainable solid-state energy storage systems.

Keywords: Sodium-Ion Batteries, composite polymer electrolyte, interfacial engineering

Evolution of Quasi-Vertically Oriented Sb_2S_3 Micropillar Arrays via Sulfurization of Sputtered Antimony Thin Films

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Abstract

Sputtered Antimony films were sulfurized at different temperatures. SEM images indicate growth of antimony-sulphide micropillars. To the best of our literature survey, these structures have not been reported yet. XRD results confirm these to be of Sb_2S_3, also, the texture coefficient indicates that these pillars are largely oriented along the [1 0 1] direction. The initial TEM study indicates these pillars to be single-crystalline. The UV-Vis spectroscopy performed on these films with pillars indicate that the band-gap is of the order for ~1.5 eV. Sb_2S_3 is a promising semiconductor for the application in photovoltaics, batteries, and photo-electrochemistry. This pillar morphology, that too pillars attached to the substrate, is very attractive, as it allows higher interface area, facile charge transport along the pillar-axis to the underlaying substrate.

Keywords: XRD, TEM, single crystalline, batteries, photovoltaics

Innovative Approaches in Burn Wound Healing: Overcoming Challenges and Advancing Care

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Abstract

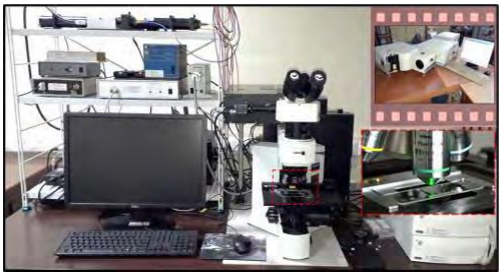
Burn wounds pose significant challenges due to their susceptibility to microbial infections, which complicates the healing process and increases the risk of mortality. Traditional treatment methods often fail to provide adequate antimicrobial protection, leading to delayed recovery and severe complications. Burn wound management has evolved significantly with the advent of bioengineered dressings designed to accelerate healing and reduce complications. Traditional dressings often fall short in providing an optimal healing environment, necessitating the development of advanced solutions. Recent innovations include hydrogel-based scaffolds, nanomaterial-infused dressings, and bioactive composites that enhance moisture retention, promote angiogenesis, and exhibit antibacterial properties. Smart wound dressings with drug-releasing capabilities and real-time monitoring sensors further revolutionize patient care. This review highlights cutting-edge advancements in burn wound dressings, addressing challenges such as infection control, biocompatibility, and clinical translation. Future research should focus on integrating regenerative medicine and personalized treatment approaches to optimize wound healing outcomes.

Keywords: Burn wound; Antimicrobial; Hydrogel; Biocompatibility

Research Facilities & Teaching Laboratories

MSE at IITK houses most of modern facilities that are required for state-of-the-art research. The department has range of equipment for materials processing, structural characterization, property evaluation, and mechanical testing. The department also has number of teaching laboratories which are also equipped with research facilities. **These facilities are primarily for the departmental research and teaching purpose. However, it is opened for the other users from other colleges, universities, research centres and industries.** Outside users can request a slot via contacting the individual faculty and lab in-charge to use the following facilities.

RAMAN AND PL SPECTROSCOPY



Raman Spectroscopy provides information of molecular vibrations, crystal structure, orientation and stress.

SCANNING ELECTRON MICROSCOPE

SEM provides topographic, phase information about the materials through SE, BSE, EBSD modes.

X-RAY DIFFRACTION FACILITY

This facility offers measurements such as ambient, high and low temperature polycrystalline XRD, Texture and residual analysis

TRANSMISSION ELECTRON MICROSCOPE

This analytical TEM provides nearly complete microstructural analysis such as imaging, micro-, nano-diffraction, CBED, lattice imaging and elemental

METALLURGICAL WORKSHOP

Modern workshop machineries such as CNC wire EDM, CNC lathe, drilling, cutting, milling etc., support for designing research apparatus & making standard specimens.

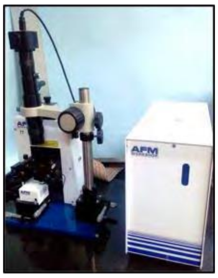
ENGINEERING METALLURGY LABORATORY

This lab equipped with various welding techniques, metal casting, sheet metal working, and typical metal deformation techniques including rolling, forging, swaging etc.

MATERIALS TESTING LABORATORY

This lab envisaged for evaluating the mechanical properties through tensile testing, hardness, creep, fatigue, impact testing etc.

MATERIALS SCIENCE LABORATORY

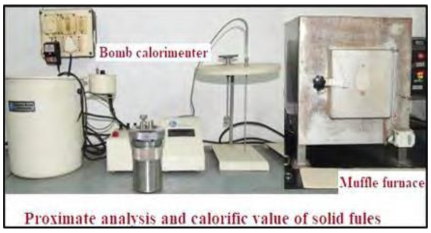


This lab includes series of experimental setup related to materials science, biomaterial, semiconductors, solar cells etc. for teaching as well as research.

PHYSICAL METALLURGY LABORATORY

This lab facilitates nearly complete metallurgical investigations including heat treatment, metallography, hardness testing, and various other facilities.

PROCESS METALLURGY LABORATORY



This lab provides insight about different mineral processing involved in ferrous and non-ferrous metal extraction.

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