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The 2nd International Electronic Conference on Metals

5–7 May 2025 | Online

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The 2nd International Electronic Conference on Metals

5–7 May 2025 | Online



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Welcome from the Chairs

Dear colleagues,

It is our pleasure to invite you to join the 2nd International Electronic Conference on Metals, which will be hosted online from 5 to 7 May 2025.

As one of the pillar technologies that support the development of modern society, metallurgy, and Metals play a crucial role in addressing major societal challenges. In recent decades with rapid technological advances, metallic materials have been extended to many emerged technological fields for a wider range of applications, not only used as structural materials but also as functional ones. IECME 2025 will present the state-of-the-art of Metallurgy and Metals related to the following topics:

- S1. Computation, AI, and Machine Learning on Metals;
- S2. Metallic Materials Chemistry;
- S3. Microstructure of Metals and Alloys;
- S4. Entropic Alloys and Meta-Metals;
- S5. Metallic Functional/ Electronics Materials;
- S6. Additive Manufacturing;
- S7. Corrosion, Wear, and Protection;
- S8. Metallic Materials Processing;
- S9. Metallic Materials for Biomedical Applications.

IECME 2025 will enable you to share and discuss your most recent research findings with the worldwide vibrant community of scientists and engineers in the field.

IECME 2025 will make your presentation accessible to hundreds of researchers worldwide, with the active engagement of the audience in question-and-answer sessions and discussion groups that will take place online.

The conference committee will review the submitted abstracts. The authors of accepted contributions will have their work displayed in an abstract collection. Following the conference, outstanding contributions will be invited to be submitted as a full-length paper for publication in *Metals* (ISSN: ISSN 2075-4701, Impact Factor 2.6).

We hope you will join us, present your work at IECME 2025, and be part of this exciting online event.



Prof. Dr. Dongyang Li
Event Chairs

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Prof. Dr. Yung C. Shin
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Journal Rank: JCR-Q2 (Metallurgy and Metallurgical Engineering) / CiteScore-Q1 (Metals and Alloys)

Rapid Publication: manuscripts are peer-reviewed and a first decision is provided to authors approximately 17.8 days after submission; acceptance to publication is undertaken in 2.7 days (median values for papers published in this journal in the second half of 2024).

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Session Chairs



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Invited Speakers



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Prof. Dr. Roberto Chiesa

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Program Overview

	Day 1	Day 2	Day 3
Morning	Welcome and Opening Remarks Event Chairs (08:50 CEST 02:50 EDT 14:50 CST) Session 9. Metallic Materials for Biomedical Applications and Keynote and Invited Talks Contributed Oral Presentations (09:00 CEST 03:00 EDT 15:00 CST)	Session 7. Corrosion, Wear, and Protection Keynote and Invited Talks Contributed Oral Presentations (09:00 CEST 03:00 EDT 15:00 CST)	Session 6. Additive Manufacturing and Session 8. Metallic Materials Processing Keynote and Invited Talks Contributed Oral Presentations (09:00 CEST 03:00 EDT 15:00 CST)
Afternoon	Session 4. Entropic Alloys and Meta-Metals and Session 1. Computation, AI, and Machine Learning on Metals Keynote and Invited Talks Contributed Oral Presentations (15:00 CEST 09:00 EDT 21:00 CST)	Session 5. Metallic Functional/ Electronics Materials Keynote and Invited Talks Contributed Oral Presentations (14:00 CEST 08:00 EDT 20:00 CST)	Session 3. Microstructure of Metals and Alloys and Session 2. Metallic Materials Chemistry and Keynote and Invited Talks Contributed Oral Presentations (14:00 CEST 08:00 EDT 20:00 CST)

IECME Program

5 May 2025 (Monday)

S9. Metallic Materials for Biomedical Applications

Time: 8:50 (CEST, Basel) | 02:50 (EDT, New York) | 14:50 (CST Asia, Beijing)

Time (CEST)	Speaker	Title
08:50–09:00	Prof. Dr. Dongyang Li and Prof. Dr. Yung C. Shin Event Chairs	Welcome and Opening Remarks
09:00–09:10	Prof. Dr. Francesca Borgioli Session Chair	Welcome by Session Chair
09:10–09:25	Prof. Dr. Roberto Chiesa Invited Speaker	Surface Treatments for Implantable Metals: Present and Future
09:25–09:40	Prof. Dr. Silvia Spriano Invited Speaker	Metal Surfaces as Interfaces with Liquids and Biological Tissues: Texturing and Functionalization for Biomolecule Release and Adsorption
	<u>Contributed Oral Presentations</u>	<u>Session 9. Metallic Materials for Biomedical Applications</u>
09:40–09:55	Hemant Kumar Pant Selected Speaker	Development of Mg-1Zn-1Ca-xZnO (x = 0 and 2 wt.%) composite using disintegrated melt deposition method for biomedical applications
09:55–10:10	Nadezhda Artyukhova Selected Speaker	Creation of thin TiNi wires with stabilized martensite phase
10:10–10:25	Elena Aldisovna Bolshevich Selected Speaker	Study of corrosion behavior of biocompatible porous monolithic material based on titanium nickelide
10:25–10:40	Amantle Balang Selected Speaker	Surface Roughness Optimization of CP Titanium for Improved Osseointegration in Dental Implants
10:40–10:55	Mina Ahmadi Selected Speaker	A review on perovskite magnetic nanoparticles (MNPs) used in magnetic hyperthermia (HT)
10:55–16:00	Break	Break

S4. Entropic Alloys and Meta-Metals and S1. Computation, AI, and Machine Learning on Metals

Time: 15:00 (CEST, Basel) | 09:00 (EDT, New York) | 21:00 (CST Asia, Beijing)

Time (CEST)	Speaker	Title
15:00–15:10	Prof. Dr. Sake Wang Session Chair	Welcome by Session Chair
15:10–15:30	Prof. Dr. Sake Wang Keynote Speaker	Two-Dimensional Valleytronic Materials: From Principles to Device Applications
	<u>Contributed Oral Presentation</u>	<u>Session 4. Entropic Alloys and Meta-Metals</u>

15:30–15:45	Isaque Moura Selected Speaker	Impact of B ₄ C on phase transformation and mechanical behavior in metastable High-Entropy Alloys
15:45–16:00	Break	Break
16:00–16:10	Prof. Dr. Chuang Deng Session Chair	Welcome by Session Chair
16:10–16:25	Prof. Liang Qi Invited Speaker	Physics-informed Machine Learning Design of Refractory Complex Concentrated Alloys for Advanced Manufacturing
	<i><u>Contributed Oral Presentations</u></i>	<u>Session 1. Computation, AI, and Machine Learning on Metals</u>
16:25–16:40	Arman Hobhaydar Selected Speaker	An Integrated Experimental and Quantum/Atomic Modelling of FeCrV-Based Refractory Medium Entropy Alloy for Nuclear Application
16:40–16:55	János György Bátorfi Selected Speaker	Effective modeling of cold rolling of metals
16:55–17:10	Zuoyong Zhang Selected Speaker	Interstitial grain boundary segregation in substitutional binary Al alloys
17:10–17:25	Mordecai Mashamaite Selected Speaker	Phase equilibrium of Ti-Pt-Nb high temperature shape memory alloys studied by cluster expansion techniques
17:25–17:40	Santiago Zapata Boada Selected Speaker	Predicting Corrosion Rate in Oil Wells Using First Principles and Machine Learning
17:40–17:55	Kseniya Utkina Selected Speaker	Prediction of the critical cooling rate in the dependence of the chemical composition of super duplex steel X03Cr23Ni6Mo4Cu3NbN

6 May 2025 (Tuesday)

S7. Corrosion, Wear, and Protection

Time: 9:00 (CEST, Basel) | 03:00 (EDT, New York) | 15:00 (CST Asia, Beijing)

Time (CEST)	Speaker	Title
09:00–09:10	Prof. Dr. Branimir Grgur Session Chair	Welcome by Session Chair
09:10–09:30	Dr. Aleksandra Popović Keynote Speaker	Influence of Alkyd Composite Coatings with Polyaniline Doped with Different Organic Acids on the Corrosion of Mild Steel
	<i><u>Contributed Oral Presentations</u></i>	<u>Session 7. Corrosion, Wear, and Protection</u>
09:30–09:45	Kamelia Blyid Selected Speaker	Optimization of Zn-Ni Alloy coating to enhance corrosion resistance of

		carbon steel Kamelia Blyid, Rida allah Belakhmima, Mohamed Ebn Touhami
09:45–10:00	Nina Kovač Selected Speaker	PMMA–Siloxane–Silica Coating to Enhance Corrosion Resistance of AZ31
10:00–10:15	Maria Andrea Reyes Reyes Selected Speaker	Microbial corrosion in oil transportation and storage systems: laboratory-scale study on biofilm and pitting formation
10:15–10:30	Luca Pezzato Selected Speaker	Functionalization of metal surfaces through plasma electrolytic oxidation (PEO) treatments with the addition of particles
10:30–10:45	Marianthi Bouzouni Selected Speaker	Investigation of Surface Oxidation Behavior on High Tensile Brass and its Effect on Hot Forging
10:45–11:00	Zakia Aribou Selected Speaker	Exploring the Influence of Polymer Additives on the Structure and Morphology of Copper Electrodeposits in Acid Sulfate Electrolytes
11:00–14:00	Break	Break

S5. Metallic Functional/ Electronics Materials

Time: 14:00 (CEST, Basel) | 08:00 (EDT, New York) | 20:00 (CST Asia, Beijing)

Time (CEST)	Speaker	Title
14:00–14:10	Prof. Dr. Juan José Suñol Martínez Session Chair	Welcome by Session Chair
14:10–14:30	Prof. Dr. Juan José Suñol Martínez Keynote Speaker	Advanced materials and Technologies in metallic materials
	<u>Contributed Oral Presentations</u>	<u>Session 5. Metallic Functional/ Electronics Materials</u>
14:30–14:45	Evgeniy D. Chernov Selected Speaker	Metallic and half-metallic properties of full Heusler alloy Co ₂ MnGa with antisite defects
14:45–15:00	Jason Daza Selected Speaker	Innovation in Manufacturing Technologies with Eco-Sustainable Magnetic Materials
15:00–15:15	Semyon Timofeevich Baidak Selected Speaker	Anomalous metallic and half-metallic properties of the Gd ₄ Sb ₃ intermetallic compound
15:15–15:30	Niclas Hanisch Selected Speaker	Ultrasonic Powder Atomization of Raney Nickel-type Precursors for Hydrogen Cathodes in Water Electrolysis

7 May 2025 (Wednesday)
**S6. Additive Manufacturing and
S8. Metallic Materials Processing**
Time: 9:00 (CEST, Basel) | 03:00 (EDT, New York) | 15:00 (CST Asia, Beijing)

Time (CEST)	Speaker	Title
09:00–09:10	Prof. Dr. Abdollah Saboori Session Chair	Welcome by Session Chair
09:10–09:25	Dr. Gabriele Piscopo Invited Speaker	Laser Deposition (DED) as an effective tool for the additive repair: basic concepts and industrial applications
	<u>Contributed Oral Presentations</u>	<u>Session 6. Additive Manufacturing</u>
09:25–09:40	Mohammad Abankar Selected Speaker	Friction stir welding of laser powder bed fusion additively manufactured aluminum and copper alloys
09:40–09:55	Sanae Tajalli Nobari Selected Speaker	Development of new stainless steel via Laser powder bed fusion process
09:55–10:10	Alireza Moradi Selected Speaker	Machine learning-assisted material development via Laser powder bed fusion process
10:10–10:25	Somnath Nandi Selected Speaker	Performance Analysis of Ni-Doped SS316L Electro-Catalysts Synthesized via Wire Arc Additive Manufacturing (WAAM)
10:25–10:35	Prof. Dr. Shusen Wu Session Chair	Welcome by Session Chair
	<u>Contributed Oral Presentations</u>	<u>Session 8. Metallic Materials Processing</u>
10:35–10:50	Jaivindra Singh Selected Speaker	Exploring the Impact of MIG Brazing Techniques on Stability, Bead Morphology, and Joint Performance
10:50–11:05	Michael Johanes Selected Speaker	The Potential Property-Tailoring Effects of Cryogenic Treatment on Pure Zinc
11:05–11:20	Mohammad Uddin Selected Speaker	Effect of synergistic burnishing–tumbling treatment on surface roughness, microstructure, hardness and mechanical strength of AISI 304 alloys
11:20–14:00	Break	Break

**S3. Microstructure of Metals and Alloys and
S2. Metallic Materials Chemistry**
Time: 14:00 (CEST, Basel) | 08:00 (EDT, New York) | 20:00 (CST Asia, Beijing)

Time (CEST)	Speaker	Title
14:00–14:10	Prof. Dr. Maria Cecilia Poletti Session Chair	Welcome by Session Chair

14:10–14:25	Dr. Safia Alleg Invited Speaker	Effect of the sintering conditions on the microstructure and mechanical properties of the high entropy alloys
	<u>Contributed Oral Presentations</u>	<u>Session 3. Microstructure of Metals and Alloys</u>
14:25–14:40	Esmail Shahryari Selected Speaker	Hot deformation mechanisms of a metastable Ti-18Mo alloy
14:40–14:55	Jiajia Shen Selected Speaker	Gas tungsten arc welding of as-cast AlCoCrFeNi ₂ . 1 eutectic high-entropy alloy
14:55–15:10	Nthabiseng Nhlapo Selected Speaker	Microstructure of as-built 3D-printed Ti and Ti64 biomaterials alloyed with copper
15:10–15:20	Prof. Dr. Michael McNallan Session Chair	Welcome by Session Chair
	<u>Contributed Oral Presentations</u>	<u>Session 2. Metallic Materials Chemistry</u>
15:20–15:35	Suneel Selected Speaker	Environmental applications of S-doped g-C ₃ N ₄ in photocatalytic degradation of Congo Red dyes under solar light Irradiation
15:35–15:50	Taimo Priinits Selected Speaker	Structural Chemistry and Crystallographic Features of Nb ₃ Sn Intermetallics
15:50–16:05	Ayob Zanberi Selected Speaker	Catalytic effects of metal (Ti) addition on the dehydrogenation properties of aluminium hydride
16:05–16:20	Omar Boualam Selected Speaker	Development of Iron/Indium-Impregnated Illite: A Novel Catalyst for Dye Degradation in Aqueous Systems
16:20–16:35	Mohammad Ismail Selected Speaker	Catalytic effects of metals (Ni and Fe) addition on the dehydrogenation properties of aluminium hydride

Session 1. Computation, AI, and Machine Learning on Metals

sciforum-114792: An Integrated Experimental and Quantum/Atomic Modelling of FeCrV-Based Refractory Medium Entropy Alloy for Nuclear Application

Arman Hobhaydar ^{1,*}, Xiao Wang ¹, Huijun Li ¹, Nam Van Tran ² and Hongtao Zhu ¹

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² School of Materials Science and Engineering (MSE), Nanyang Technological University in Singapore

Introduction

Rising energy demands and environmental challenges necessitate advancements in nuclear reactor materials to endure harsh conditions, including high temperatures, neutron flux, and oxidation. Medium-entropy alloys (MEAs) offer promising properties like enhanced strength, ductility, and radiation resistance. This study focuses on designing FeCrV-based refractory MEAs for nuclear applications using multi-scale modelling and experimental validation, leveraging the potential of DFT and machine learning to optimize performance and simulate large-scale behaviours.

Methods

First-principle calculations were performed using VASP, employing the PAW method and PBE-GGA for accurate modelling. AIMD simulations with a 0.5 fs timestep generated training data under constant and increasing temperatures. Neural network potentials were trained using DeepPot-SE. Large-scale MD simulations applied periodic boundaries and NPT equilibration at 300 K-1023 K. MC/MD methods facilitated atom exchanges, governed by Boltzmann probability, to explore temperature-dependent behaviours and structural evolution.

Results

XRD and TEM microstructure analyses revealed that the RMEA comprises two distinct phases: BCC1, the nominal alloy phase, and BCC2, a vanadium-rich phase. These two phases were also identified in MD/MC simulations conducted using the DNNP, demonstrating the accuracy of the model. The addition of 8% W to FeCr₂V significantly enhances its mechanical properties, achieving an ultimate compression strength of 1700 MPa and a Young's modulus of 255.28 GPa. According to the DFT results, these improvements are attributed to a balanced interaction between metallic and covalent bonding, producing a highly irradiation-resistant material with an average vacancy formation energy of 2.66 eV. Dislocation analysis conducted via MD revealed that increasing the temperature enhances dislocation mobility, which further improves the ductility of the alloy.

Conclusion

In conclusion, a cost-effective FeCr₂V-based RMEA with superior mechanical properties, including high strength, ductility, and irradiation resistance, was successfully designed. With properties surpassing HEAs, this alloy demonstrates improved dislocation mobility at elevated temperatures, highlighting its potential for advanced structural applications in extreme environments.



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sciforum-112784: Data Science and Numerical Simulations: Shaping the Future of Metal Process Modeling

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Abstract

With the emergence of data science techniques, such as reduced-order schemes, real-time modeling, machine learning (ML), and smart control schemes, material process modeling and simulations are undergoing a revolutionary phase. Although traditional analytical methods and advanced numerical simulations still provide estimations of multi-physical and multi-scale material processes, generating real-time predictions remains challenging for these techniques. Additionally, data quality and availability issues have slowed the development of data models, while long computational times have hindered the use of advanced numerical simulations for process control. This paper presents the outcomes of research on the simultaneous use of data models and detailed numerical simulations, highlighting their unique roles in control and data generation for future process modeling. While many data processing and handling schemes exist within the data science field, only a few are suitable for material process applications due to their transient and multi-physical natures. As more physics and phases are considered in numerical simulations, the computational time and resources required become enormous, even for today's parallel and clustered computers. Recently, integrating certain data techniques within numerical simulation frameworks has drastically reduced computational time (e.g., recurrence computational fluid dynamics). This research scrutinizes the efficient use of these simulation techniques for creating fast databases and utilizing these databases for real-time predictions in transient material processes (e.g., casting processes). Consequently, both data models and numerical simulations, along with experimental validations, play crucial roles in generating accurate and reliable metal process modeling. The objective is to integrate these techniques into digital twin and shadow frameworks, driven by industrial digitalization, to enhance greener and more efficient manufacturing. Finally, predefined simulation scenarios were used to produce reliable data models for accurate real-time predictions in metal casting process optimization and control.



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sciforum-110245: Effective modeling of cold rolling of metals

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In this work, we extended an existing version of the Flow-Line Model (FLM) to the symmetric cold rolling of technically pure aluminum sheets. Through the modifications, the rolling process can be described with improved precision even in special conditions. The FLM aims to approximate the velocity values at each point of the rollgap using the new analytical function. The difficulty of the FLM models is in finding the correct value of the parameters based on the geometrical dimensions and frictional conditions. Besides the theoretical changes to the model, a set of empirical parameters were introduced, and the equations to determine the value of these empirical parameters were built up based on numerical results of Finite Element Model (FEM) simulations for a wide range of geometrical parameters.

The main theoretical challenge is to approximate the rollgap using a proper function. The distribution of the shear strain rates along the sheet's thickness was approximated by a power function. The newly introduced empirical parameters were determined by using three non-dimensional factors: (i) the ratio of the actual to minimal coefficient of friction, (ii) the relative reduction in the sheet's thickness, and (iii) a geometrical ratio expressing the ratio of the rollgap's length to the sheet's thickness.

The model was tested for the following regimes of the non-dimensional factors: the thickness reduction was changed from 0.01 to 0.38; the ratio of the pressed arc to the radius was varied between 0.0082 and 0.31; and the ratio of the real to minimal coefficient of friction was changed from 1.05 to 2.5.

The model's precision determined from the three measured distortion lines (generated by Vickers indentations) was compared to their simulated version.



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sciforum-112814: Interstitial grain boundary segregation in substitutional binary Al alloys

Zuoyong Zhang * and Chuang Deng

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Solute segregation at grain boundaries (GBs) has emerged as a promising strategy for alloy design. While most previous studies on GB segregation have assumed that solute atoms occupy substitutional sites within GBs, recent first-principles studies have revealed that undersized elements, such as Ni, Cu, and Fe, can also segregate to hollow interstitial sites in certain Al symmetric-tilt GBs. In this study, we employ hybrid molecular dynamics (MD)/Monte Carlo (MC) simulations to investigate the segregation behavior of Ni in Al coincidence-site lattice (CSL) GBs. The results demonstrate that Ni atoms preferentially segregate to interstitial sites within the kite-like GB structures in Al CSL GBs. Building on these findings, we develop a robust method to systematically identify potential interstitial sites at CSL GBs. This method consists of two main steps: detecting candidate interstitial sites and filtering them based on their structural properties. The identified interstitial sites show a distribution that is consistent with the results of hybrid MD/MC simulations. By applying this method to nanocrystalline alloys, we calculate the interstitial segregation energies, significantly improving the accuracy of GB segregation predictions. Furthermore, machine learning models using smooth overlap of atomic positions (SOAP) descriptors successfully predict these segregation energies. This study underscores the importance of GB interstitial segregation in enhancing our understanding of solute behavior and provides valuable guidance for the design of advanced metal alloys.



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sciforum-111509: Intrinsic grain boundary mobility tensor from three-dimensional interface random walk

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In recent years, studies have demonstrated that grain boundary (GB) migration is a three-dimensional (3D) process, characterized by a 3D mobility tensor. In this presentation, we introduce a recently developed 3D interface random walk theory, which provides a framework for extracting intrinsic GB mobility and shear coupling tensors based on the random walk behavior of GB positions. This theory enables a mathematical proof of the symmetry of the GB mobility tensor in the case of overdamped GB migration. The theory and its conclusions align with molecular dynamics simulation results, and the computed shear coupling aligns closely with predictions from disconnection analysis. Additionally, we propose the fast-adapted random walk (FAIRWalk) method, enabling the efficient extraction of the GB mobility tensor from fewer simulations while maintaining high accuracy. Building on this advancement, we conducted an extensive survey of the mobility, shear coupling, and activation energy of the migration of 388 coincidence-site lattice Ni GBs in the Olmsted database. Several intriguing phenomena were observed, including temperature-induced sudden emergence, disappearance, or inversion of shear coupling; GBs with "zero" normal mobility but high shear mobility; and a non-linear relationship between activation energy and mobility. These findings challenge the traditional understanding of GB migration and warrant further investigation.



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sciforum-113779: Optimization of Copper (II) leaching process using machine learning approaches

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Using machine learning approaches such as the artificial neural network (ANN) model, the factors influencing the leaching of copper from contaminated soil using sulphuric acid were determined. The feed-forward back-propagation (BP) algorithm was used for the development, training, and prediction of the artificial neural network model. The pH of the solution, acid concentration, soil-to-liquid ratio, and stirring speed were used as input variables, while the amount of copper (II) leached was used as the output. To build and train the model, 21 datasets were taken from the leaching experiments. We looked at neural networks with one to nine hidden layers to find the one with the best agreement and to find the one that could reduce the discrepancy between the predicted and measured values. A proportion of 70% of data were used for training, 15% for testing, and 15% for validation. During the regression analysis of the four inputs, nine hidden layers, and one output design, the R^2 value for training was 0.997, that for validation was 0.996, and that for testing was 0.997. The algorithm used was Levenberg–Marquardt with membership 11-11-11-11. The corresponding MSE values were 0.121, 0.133, and 0.105. The findings indicate that the artificial neural network holds great promise for predicting the leaching of copper (II). The results showed that the ANN model's performance improved as the number of hidden layers increased.



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sciforum-115123: Phase equilibrium of Ti-Pt-Nb high-temperature shape memory alloys studied using cluster expansion techniques

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The effect of adding Nb on TiPt high-temperature shape memory alloys (HTSMAs) was investigated using the universal cluster expansion and first-principle approach. In this study, cluster expansion was utilized to predict ground state structures containing three (3) elements: Ti, Pt, and Nb. The cluster expansion method generated 45 new Ti-Pt-Nb structures, and these were ranked as stable and meta-stable structures based on their formation energies. Among the six (6) predicted structures, the $\text{Ti}_4\text{Nb}_2\text{Pt}_2$ system was selected around 50:50 on Platinum (Pt)-rich sites since it is the most stable structure on the ground state line. The supercell approach in MedeA (VASP) was used to create large supercells of about 64 atoms. In addition, the $\text{Ti}_4\text{Nb}_2\text{Pt}_2$ system was studied further by determining the structural, thermodynamic and mechanical properties using the first-principle density functional theory. The $\text{Ti}_4\text{Nb}_2\text{Pt}_2$ system was found to be the most thermodynamically stable structure due to its negative heat of formation (-0.361 eV/atom). The materials have similar properties as tetragonal Nb-doped TiPt. The mechanical properties of these compounds revealed that they are ductile in nature and mechanically stable. Furthermore, the phonon dispersion curves showed the vibrational stability of the $\text{Ti}_4\text{Nb}_2\text{Pt}_2$ alloy due to the absence of soft modes. This work suggests that introducing Nb stabilizes the TiPt SMAs, making them potential candidates for high-temperature applications.



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sciforum-118892: Predicting Corrosion Rate in Oil Wells Using First Principles and Machine Learning

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Corrosion in oil wells results from the interaction of factors such as chemical composition, temperature, pressure, and fluid flow. Accurately predicting corrosion rates is crucial for operational efficiency and risk mitigation. Traditional models often have limitations in adapting to new operating conditions and capturing complex interactions between variables, while machine learning models can uncover these interactions. This study aims to develop a hybrid model that combines physical and chemical understanding of corrosion with machine learning approaches. Integrating fundamental corrosion principles with machine learning adaptivity, the model seeks to improve accuracy in predicting corrosion rates, thereby reducing operational costs, downtime, and safety risks. The methodology we applied began with the collection of historical data from a representative set of oil wells (more than 30,000 logs), including corrosion rates, well operating parameters, tubing parameters, and fluid compositions. The dataset was carefully cleaned and transformed, addressing missing values and outliers. To integrate first principles, the NORSOK corrosion model, based on fundamental chemical and physical concepts, was applied to calculate theoretical corrosion rates. Subsequently, machine learning models—such as Linear Models, Bootstrap Forest, and Boosted Tree—were trained using metrics like RSquare and Mean Average Error (MAE) to evaluate performance. Among the tested models, a Boosted Tree model (XGBoost) achieved the best performance, achieving an RSquare of 0.163 and an MAE of 1.39, capturing complex parameter relationships. Incorporating the NORSOK-based first principles ensured the model remained robust under varying conditions. Finally, a hybrid approach combining predictions from both physics- and chemistry-based and machine learning models was deployed in the cloud for real-time corrosion rate predictions. This deployment offers significant cost savings—up to a 30% reduction in chemical treatment costs—and enhances operational efficiency by minimizing downtime due to corrosion events.



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sciforum-117485: Prediction of the critical cooling rate in the dependence of the chemical composition of super duplex steel X03Cr23Ni6Mo4Cu3NbN

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Introduction

Super duplex steel 03Cr23Ni6Mo4Cu3NbN (SDS) is a new development of JSC "NPO 'TSNIITMASH', which has high corrosion and strength characteristics which are in demand in the oil and gas industries, as well as in chemical industry and nuclear power engineering. The combination of these characteristics is ensured by uniform distribution of austenite and ferrite. Special attention is paid to the technology of ingots and forgings manufacturing, prevention of formation and growth of σ -phase, and other secondary phases which negatively affect the mechanical and operational properties of steel. The influence of chemical composition and technological parameters, including ingot solidification and forgings cooling rates, on structure formation is investigated using computer modeling and experimental studies.

Methods

- Modeling of phase transformations of 1000 chemical compositions is carried out using the program complex Thermo-Calc version 2022a (with PRISMA) using databases TCFE11, MOBFE6.
- Production of 03Cr23Ni6Mo4Cu3NbN steel samples takes place using electroslag remelting (ESR) with the provision of increased crystallization rates. The cooling rates from 2.5 to 42 °C/s are realized when the forgings are quenched.
- The chemical composition, microstructure, and impact toughness of steel are determined.

Results

The influence of alloying elements and cooling rate of forgings on the kinetics of σ -phase formation is described on the basis of computer modeling. Parametric models approximating the results of thermodynamic and kinetic calculations are developed. The models allow us to calculate the fraction of σ -phase at given cooling rates to estimate the value of impact toughness of steel.

Conclusions

On the basis of regression analysis, the influence of nitrogen, molybdenum, nickel, copper and carbon on the value of critical cooling rate has been established.

The equation for calculation of impact toughness depending on the volume fraction of σ -phase has been proposed.

The possibility of preventing the growth of complex nitrides of CrNbN system, negatively affecting the impact toughness, by controlling the conditions of solidification at ESR has been established.



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sciforum-113780: Soft computing model application for the modelling and prediction of copper (II) leaching

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Optimising the parameters of leaching while assessing the dynamics of the process kinetics requires an investigation of the effects of different variables. A neural network (NN) and a fuzzy inference system (FIS) were used to evaluate and examine the leaching process. The results showed that increasing the acid concentration and stirring speed, while decreasing the solid-to-solution ratio and pH, enhanced copper (II) leaching. The optimum values obtained from the leaching process for pH 3 were found to be a solid-to-liquid ratio of 1g/100 mL, an agitation speed of 300 rpm, and an acid concentration of 1 M, with a 97% recovery of copper (II). Diffusion throughout the product layer controlled the leaching rate, and the experimental results suggested that a diffusion-controlled model would provide the best fit. The diffusion-controlled mechanism was indicated by an activation energy of 16.01 kJ/mol. To optimise the parameters of the leaching process, the algorithm training for neural networks (NNs) included the Levenberg–Marquardt method with a membership structure of 7-7-7-7, using the backpropagation (BP) technique for learning. The neural network (NN) method was trained using four input variables, representing leaching parameters, fifteen hidden layers, and one output representing copper (II) leaching recovery. R^2 values of 0.996, 0.997, and 0.997, respectively, show the validation, testing, and training phases of the ideal trained neural network. An R^2 value of 0.999 for FIS indicates that the study data can be precisely predicted. ANFIS had a Pearson's chi-squared value of 0.225, surpassing the ANN's score of 0.658.



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sciforum-114565: The Performance of Hybrid R/C-Steel Structures under Successive Earthquakes

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In the conventional building procedure, numerous circumstances may be discovered regarding building types composed of a lower and older reinforced concrete (r/c) component and an upper and newer steel part, referred to as a "hybrid" building. Established principles of seismic design provide comprehensive instructions for the resistant design of structures built using a single material everywhere. The present seismic norms do not give explicit design and detailing requirements for vertical hybrid structures. There needs to be more investigation in existing research, addressing this scientific gap. The current study attempts to fill this knowledge gap on hybrid construction performance under successive ground motions, which have been reported in research worldwide in terms of seismic structural performance. Three-dimensional representations of hybrid r/c-steel building frames are subjected to successive ground stimulations across the horizontal and vertical directions, implementing a non-linear response of the frame components over time. The bottom r/c part of the hybrid structures is described as relating to a previous construction using an essential approximation here. Furthermore, two limit interconnections of the structural steel component to the concrete one are identified for investigation in non-linear time history analysis. An evaluation of the arithmetic analysis outcomes of the hybrid frames considering the two limit interconnections is performed. The analysis diagrams of the present dynamic investigations of the 3D hybrid frames exposed to successive ground motions provide helpful insights that offer guidelines for a better earthquake-resistant design of the "hybrid" building form, which does not fall within the scope of the present standards despite being frequently used.



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Session 2. Metallic Materials Chemistry

sciforum-114944: Catalytic effects of metal (Ti) addition on the dehydrogenation properties of aluminium hydride

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Due to its high hydrogen capacity (10.1 wt.%), aluminium hydride (AlH_3) is considered as a possible material for on-board hydrogen storage applications. However, several factors, such as a high decomposition temperature and sluggish desorption kinetics, limit this benefit and render this material unmarketable. To overcome these limitations, numerous studies have been conducted, such as using mechanical ball milling to reduce the particle size and adding dopants or catalysts. In this work, the effect of metal (Ti) on the dehydrogenation properties of AlH_3 has been investigated for the first time. The results show that Ti lowered the initial decomposition temperature and sped up the process of AlH_3 desorption. The 10 wt.% Ti-doped AlH_3 sample's initial decomposition temperature dropped from 145 °C to 120 °C compared to that of as-received AlH_3 . For the desorption kinetic measurements at 100 °C, the 10 wt.% Ti-doped AlH_3 sample could desorb about 4.0 wt.% of H_2 in 20 min compared to 0.1 wt.% for the as-received AlH_3 . After Ti was added, the activation energy for the dehydrogenation process of AlH_3 that was determined by Kissinger analysis decreased. From the X-ray diffraction analysis, we found that Ti did not react with AlH_3 during the mechanical milling and heating (desorption) processes. Ti is believed to play a catalytic role by inducing Ti-H interaction and weakening Al-H bonding, thus improving the dehydrogenation properties of AlH_3 .



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sciforum-112133: Catalytic effects of metals (Ni and Fe) addition on the dehydrogenation properties of aluminium hydride

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Due to its large hydrogen capacity (10.1 wt.%), aluminium hydride (AlH_3) is considered as a possible material for on-board hydrogen storage applications. However, several factors, such as its high decomposition temperature and sluggish desorption kinetics, limit this benefit and render this material unmarketable. To overcome these limitations, numerous studies have been conducted, such as using mechanical milling to reduce the particle size and adding dopants or catalysts. In this work, the effect of metals (Ni and Fe) on the dehydrogenation properties of AlH_3 has been investigated for the first time. The results show that Ni is a better catalyst than Fe when it comes to lowering the initial decomposition temperature and speeding up the process of AlH_3 desorption. The 10 wt.% Ni-doped AlH_3 sample's starting decomposition temperature dropped from 130 °C to 80 °C compared to that of as-milled AlH_3 . In the desorption kinetic measurements at 100 °C, the 10 wt% Ni-doped AlH_3 sample desorbed about 6.7 wt% of H_2 in 20 min compared to the 4.5 wt% desorption exhibited by the as-milled AlH_3 . After Ni was added, the activation energy for the dehydrogenation process of AlH_3 that was determined by Kissinger analysis was decreased. From the X-ray diffraction analysis, we found that Ni did not react with AlH_3 during the mechanical milling and heating (desorption) processes. Ni is believed to play a catalytic role by inducing Ni-H interaction and weakening Al-H bonding, which improves the dehydrogenation storage properties of AlH_3 .



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sciforum-112410: Development of Iron/Indium-Impregnated Illite: A Novel Catalyst for Dye Degradation in Aqueous Systems

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The application of metallic materials in environmental remediation has gained increasing attention due to the need for sustainable solutions to pollution. This study investigates the preparation and application of illite impregnated with iron (Fe) and indium (In) as a heterogeneous catalyst for the degradation of malachite green, a persistent and toxic dye used in industrial processes.

The Fe/In-impregnated illite catalyst was synthesized using a wet impregnation method, enabling the effective incorporation of metal ions into the clay matrix. Advanced characterization techniques, including X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and scanning electron microscopy with energy-dispersive X-ray analysis (SEM-EDX), were employed to confirm the structural and compositional modifications.

The catalytic activity of the synthesized material was evaluated through dye degradation experiments under varying reaction conditions, such as pH, dye concentration, and temperature. The results demonstrate that the Fe/In-illite catalyst achieved a degradation efficiency exceeding 97% for malachite green under optimal conditions. The kinetic studies revealed a pseudo-first-order reaction mechanism, highlighting the synergistic effect of iron and indium in enhancing the oxidative degradation process.

This work underscores the potential of combining metallic chemistry with natural clays to develop cost-effective and eco-friendly catalysts. The findings contribute to advancing the field of metallic materials chemistry for environmental and industrial applications.



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sciforum-119420: Environmental applications of S-doped g-C₃N₄ in photocatalytic degradation of Congo Red dyes under solar light Irradiation

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Background:

Today, researchers are focusing on preparing photoactive semiconductor materials doped with non-metals; such semiconductors may be considered a prospective route to resolving the worldwide water crisis by degrading organic dyes present in wastewater from the textile industry.

Methodology, results, and conclusions:

Herein, we report a facile route to synthesise S-doped graphitic carbon nitride (S-GCN) from thiourea via thermal polymerisation methods. The crystalline nature of the synthesised photocatalyst was examined by utilising X-ray diffraction (XRD), with the peak positions at Bragg angles (2 θ) of 13.07° and 27.42°, which correspond to Miller indices of (100) and (002), respectively; however, their functional group purity was evaluated through Fourier transform spectroscopy (FT-IR), and the presence of three distinct bands appearing at 3153 and 1636-1240 indicates the presence of N-H and O-H stretching modes of heterocyclic S-doped g-C-N, whereas the region between 805 and 812 cm⁻¹ represents the tri-s-triazine unit of S-GCN. All these results indicated that the synthesised photocatalyst exhibited good crystallinity and purity. To examine the photocatalytic activity, 0.2 g/L of synthesised S-GCN was immersed in 100 mL of 10 ppm Congo red dye solution, stirred for 25 minutes, and kept in the dark to establish adsorption-desorption equilibrium followed by open sunlight irradiation. During irradiation, a 3 mL suspension was taken out at intervals of 25 minutes; absorbance was measured, which decreased with time. Moreover, the S-doped GCN displayed good photocatalytic activity in 150 min of sunlight exposure. The degradation of dyes followed pseudo-first-order kinetics.



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sciforum-114409: Pristine and Pt-Modified TiO₂ Drive Organic Compound Photodegradation

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Introduction:

Sunlight-induced photocatalytic oxidation of organic matter is significant for a number of reasons, including (i) its low cost, (ii) its ability to purify air and water [1], and (iii) its role as an alternative to the selective synthesis of high-value oxygenated compounds [2].

Methods:

Materials used: ethanol, TiO₂, and Pt/TiO₂ powders (obtained by sol-gel method). The reaction products of gas-phase oxidation processes were analyzed by gas-phase chromatography (GC-TCD and GC-FID).

Results:

Considering light-induced ethanol oxidation on a noble metal (Pt) loaded with TiO₂, both the support and noble metals are crucial for light absorption, charge separation, and carbon dioxide generation. Platinum nanoparticles on TiO₂ can primarily cause the separation of photogenerated charges and a red shift in the light absorption edge.

Figure 1. Oxidative conversion of ethanol driven by solar light.

Conclusions:

The light-initiated photo-oxidative routes of an organic substrate over TiO₂ charged with noble metals are revealed in this study. The production of carbon dioxide, the separation of the light-generated charges by platinum addition, and the mechanism of the oxidative conversion reaction of ethanol are the main topics of this analysis of the intricate phenomena connected to the photocatalytic processes.

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sciforum-119366: Structural Chemistry and Crystallographic Features of Nb₃Sn Intermetallics

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The use of binary A15 systems as low-T_c superconductors is of great importance for the development of many modern engineering and technological solutions. As a typical representative of this family, we chose the Nb₃Sn system for our structural studies. Our presentation will focus on two main results: The first is the atomic-scale modeling of Nb chain formation in the condensation of the 3:1 binary combination of Nb and Sn atoms. We will discuss reconstruction in the context of the symmetry of the cubic structure, specifically the transformation of the bcc-type superlattice with Im-3m space symmetry and the crystal phases arising along the Im-3m→Pm-3n symmetry-lowering pathway. We argue that, when Nb and Sn are condensed as Nb₃Sn in the Pm-3n cubic structure, the stabilization of the chains of Nb atoms running parallel to the main cubic axis is caused by their periodic off-center displacements. Change in the point symmetry of the Nb positions is a necessary condition for stable charge ordering. The other effect we will discuss relates to the crystallographic orbits of the Nb sites in the Nb₃Sn Pm-3n lattice geometry. The point symmetry microstructure is caused by the 6c→6d shift in the change of occupation of the 6c Wyckoff positions. Such an occupation shift induces the phenomenon of structural modulation between niobium chain orientations and, thus, defines the bulk structure as composed of subsystems, where the orientation of the niobium chains induces anisotropy caused by the distinct chain patterning in the neighboring lattice regions. Translational symmetry of the Pm-3n space group begins to hold only through the partitioned subsystems. This allows us to predict that the crystallographic equivalence in the point symmetry of Nb sites may be removed when the alloy microstructure is assembled as adjacent grains.



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Session 3. Microstructure of Metals and Alloys

sciforum-116039: Gas tungsten arc welding of a multiphase CoCuFeMnNi high-entropy alloy

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Since their inception, high-entropy alloys (HEAs) have been the subject of an increasing amount of research involving a plethora of compositions and environmental conditions. In line with this, research on their processability is crucial to achieve competitive alternatives to common engineering alloys for potential structural and functional applications. For such endeavors, gas tungsten arc welding (GTAW), which is widely used in industry to obtain monolithic parts from separate components, is capable of supplying pertinent information regarding the feasibility of combining new materials in terms of their microstructure and mechanical performance.

With this in mind, in the present work, we present an analysis of the feasibility of GTAW of CoCuFeMnNi HEA. This is accomplished by delving into microstructural observations using conventional and advanced techniques, such as synchrotron X-ray diffraction coupled with CalPhaD-based calculations, to fully comprehend the microstructure across the weld. The mechanical performance of the joints is also researched in terms of microhardness and tensile testing.

Overall, the dual-phase nature of the HEA is observed throughout the welded joint, where the nucleation of a B2 BCC phase is highlighted in the heat-affected zone. The obtained joints however, exhibit poor mechanical performance, which is attributed to the residual stresses and sizeable grains which develop within the solidifying molten pool.



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sciforum-120007: Hot deformation mechanisms of a metastable Ti-18Mo alloy

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Metastable molybdenum (Mo)-based titanium alloys exhibit a low Young's modulus, along with excellent biocompatibility, corrosion resistance, and mechanical properties, making them ideal for biomedical applications. The microstructure of Ti-Mo alloys can be tailored through thermomechanical processing, where Mo diffusion significantly influences microstructural evolution. To investigate the deformation mechanisms of a Ti-18Mo alloy, hot compression tests were performed using a Gleeble® 3800 in both the $\alpha+\beta$ - and β -phase regions at temperatures ranging from 610 °C to 910 °C and strain rates between 0.01 s⁻¹ and 10 s⁻¹, reaching final strains of 0.50 and 0.80, followed by an immediate water quench. Scanning electron microscopy images and electron backscatter diffraction measurements were used to examine the microstructure of the deformed samples in the $\alpha+\beta$ - and β -phase regions, respectively. In the β -phase region, the flow curves exhibit a broad work hardening, uncommon in various β -Ti alloys, representing a slowing of dynamic restoration processes, likely due to the influence of Mo on the softening kinetics. Flow curves from $\alpha+\beta$ -phase deformation show a softening after the peak value, attributed to the globularisation of the α phase. Heterogeneous microstructures were observed during deformation in both regions, indicating that the subgrain formation and α phase globularisation primarily occurred near the previous grain boundaries. Dynamic recovery, dynamic recrystallisation, subgrain size, and α phase globularisation were quantified and correlated with deformation parameters and the influence of Mo.



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sciforum-116090: Gas tungsten arc welding of as-cast AlCoCrFeNi_{2.1} eutectic high-entropy alloy

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AlCoCrFeNi_{2.1} eutectic high-entropy alloy stands out for its remarkable mechanical properties, offering an excellent balance between strength and plasticity. For the first time, gas tungsten arc welding (GTAW) was applied to this as-cast alloy to investigate its weldability and associated microstructural evolution. A comprehensive analysis of the welded joint's microstructure was performed using electron microscopy, electron backscatter diffraction (EBSD), synchrotron-based X-ray diffraction (SXRD), and thermodynamic simulations. The alloy's mechanical properties were characterized through microhardness mapping and tensile testing, which was integrated with digital image correlation (DIC) to provide insights into local deformation behavior. The welded joint, comprising the base material (BM), heat-affected zone (HAZ), and fusion zone (FZ), retained a eutectic structure with FCC and B2-type BCC phases. Variations in phase proportions arose due to thermal cycling during welding. BCC nanoprecipitates present in the BM were partially dissolved near the FZ boundary within the HAZ. Grain refinement in the FZ, driven by rapid solidification, contributed to increased hardness in this region. Despite these microstructural changes, tensile testing showed that the joints exhibited a favorable balance between strength and ductility, with failure consistently occurring in the BM. This work highlights the feasibility of using arc-based welding methods for high-entropy alloys, underscoring their potential for advanced structural applications.



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sciforum-115199: Microstructure of as-built 3D-printed Ti and Ti64 biomaterials alloyed with copper

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The use of titanium (Ti) and its alloys (particularly Ti6Al4V, or simply Ti64) to additively manufacture implants for tissue engineering in the biomedical field has seen a steep rise in recent years. Titanium is the preferred metal for bioengineering applications due to its outstanding specific strength, biocompatibility, and corrosion resistance. Additive manufacturing (AM, also known as 3D printing) provides unchallenged freedom for designers, allowing them to fabricate custom objects while maintaining a short turnaround time. The layer-by-layer production nature of 3D printing techniques, such as direct metal laser sintering (DMLS), has been successfully utilized by the medical industry to manufacture complex shapes using biocompatible materials in order to produce implants. The drawback of Ti and its alloy is that they do not innately possess antibacterial properties and may attract bacterial attachment because of their biocompatibility. Copper (Cu) is an essential mineral which displays a highly efficient antibacterial effect. Thus, alloying Ti-based implant material with Cu particles induces a bactericidal feature in such biomaterials. This paper describes the DMLS manufacturing of in situ alloyed commercially pure titanium (cpTi) and Ti6Al4V ELI with Cu and the examination of their microstructure. Studying the microstructure of 3D-printed parts is essential for predicting their mechanical properties and functionality.



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Session 4. Entropic Alloys and Meta-Metals

sciforum-111734: Impact of B₄C on phase transformation and mechanical behavior in metastable High-Entropy Alloys

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Metastable high-entropy alloys (HEAs) represent a significant advancement in material science, addressing the longstanding challenge of balancing strength and ductility in alloys. The study of metastable HEAs offers a valuable framework for exploring the influence of γ -f.c.c. $\rightarrow\epsilon$ -h.c.p. phase transformations on mechanical performance, particularly concerning volumetric changes during deformation. Structural changes, such as variations in the c/a ratio, provide critical insights into the interplay between phase stability and mechanical behavior in HEAs. We investigated the microstructure, mechanisms underlying phase transformations, and mechanical behavior of metastable Fe₄₀Mn₂₀Co₂₀Cr₁₅Si₅ and Fe₄₀Mn₂₀Co₂₀Cr₁₅Si₅ + 0.25wt.% B₄C HEAs fabricated via laser powder bed fusion (LBPF). Special attention was given to comparing how the presence of B₄C affects phase transformations, including variations in the c/a ratio, volumetric changes, and overall phase stability during deformation. The HEAs without B₄C demonstrated an increase in the c/a ratio, primarily due to a significant expansion of the c-axis, while introducing B₄C altered this response, leading to a decrease in the c/a ratio. This reduction was driven by a contraction of the c-axis rather than an expansion. Furthermore, the a-axis remained unchanged for both alloys. The contrasting behaviors highlight how adding B₄C fundamentally alters the stress-induced dimensional changes during the γ -f.c.c. $\rightarrow\epsilon$ -h.c.p. phase transformation.



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Session 5. Metallic Functional/ Electronics Materials

sciforum-114902: Analysis of the capture of microplastics with hydrophobic metallic particles

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One of the main environmental problems is related to the generation of micro- and nanoplastics. This study aims to analyze the viability of an innovative method consisting of the adsorption of microplastics using hydrophobic metal particles, which require their functionalization. A laboratory protocol (of the adsorption process) and analysis (of the particles and the adsorption efficiency) were designed. For the production of the metal particles (of micrometric size), the ball milling technique was used. Also, milling equipment operating with liquid nitrogen was used to generate the microplastics. For morphological characterization, electron microscopy was used; for structural X-ray diffraction to analyze the composition, X-ray dispersion spectroscopy was used; and to monitor the functionalization, Fourier transform infrared spectroscopy was used. The functionalization was carried out in a 1M solution of lauric acid. The metallic particles are nanocrystalline (crystallite size range of 12–44 nm) and the crystallographic phase is the bcc-Fe. It was found that the adsorption of microplastics is more efficient when the size of the metal particles is smaller. The correct functionalization of the metal particles prevents their oxidation in aqueous media. Regarding the efficiency in the capture of microplastics, the highest value found is close to 90%, depending on the metallic particle production conditions. Additional studies are needed to optimize the efficiency of microplastic capture, probably by increasing the surface/volume ratio of metal particles.



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sciforum-114820: Anomalous metallic and half-metallic properties of the Gd_4Sb_3 intermetallic compound

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The electronic structure of the Sb-based intermetallic compound Gd_4Sb_3 has been studied, and it was recently revealed to have half-metallic properties [1]. Experimentally, anomalous Nernst and Hall effects were also found in Gd_4Sb_3 , which confirmed the half-metallic behavior and anomalous electronic structure of this intermetallic compound [2]. Our calculations were performed according to an ab initio GGA+U method, which accounted for the strong electron correlations in the 4f shell of Gd. The ferromagnetic ordering in Gd_4Sb_3 is characterized by the large magnetic moment equal to $31 \mu_B$ / f. u., which is mostly formed by the magnetic moments of the Gd ions. The band structure of Gd_4Sb_3 has interesting features which were revealed by our spin-polarized calculations. We found that one spin projection had completely metallic properties with multiple bands crossing the Fermi energy, whereas the other one was found to have an energy gap of 0.67 eV. Such features are absent in the binary semimetallic GdSb or metallic GdSb_2 compound with the close composition, which makes Gd_4Sb_3 a new, interesting half-metal ferromagnet with full spin polarization [1]. This research was supported by the Russian Science Foundation pr. No. 22-42-02021.

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sciforum-119493: Cobalt-Based Electrocatalysts: A Pathway Toward Cost-Effective and High-Performance Energy Conversion

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The significant demand for sustainable and cost-effective energy solutions has led to extensive research into non-noble and earth-abundant metal-based electrocatalysts for energy conversion reactions, such as hydrogen evolution reactions (HERs). While noble metals such as platinum (Pt) and iridium (Ir) have historically dominated due to their exceptional catalytic performance, palladium (Pd) has emerged as a compelling alternative. This is primarily due to its comparatively lower cost, excellent hydrogen adsorption and desorption properties, high catalytic activity, and improved durability. Recent strategies, such as Pd-based alloying with non-noble metals (e.g., Ni, Co, Mo) and nanostructuring techniques, have resulted in enhanced catalytic performance, greater active site exposure, and better stability in alkaline conditions. Herein, cobalt-phosphorus (CoP) and cobalt-iron-phosphorus (CoFeP) coatings were deposited on the copper (Cu) substrate using an electroless deposition method. The incorporation of Pd nanoparticles on the CoP and CoFeP coatings using the galvanic displacement method has been shown to enhance the catalytic activity of the coatings. The morphology, structure, and composition of the catalytic materials were thoroughly examined using scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS), X-ray diffraction (XRD), and inductively coupled plasma optical emission spectroscopy (ICP-OES). Moreover, the electrocatalytic activity of the catalysts for the HER in an alkaline solution (1 M KOH) was studied using linear sweep voltammetry (LSV). Electrochemical measurements revealed that PdCoFeP exhibited superior HER activity with a lower overpotential of 180 mV at 10 mA cm⁻² compared to PdCoP due to synergistic effects between Pd, Fe, and Co, which promote efficient charge transfer and reduce the reaction overpotential. This work highlights that Pd-based non-noble metal electrocatalysts have the potential to accelerate the transition towards sustainable hydrogen production, thus contributing to the broader goal of clean and renewable energy technologies.

Acknowledgement

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sciforum-114901: Innovation in Manufacturing Technologies with Eco-Sustainable Magnetic Materials

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In the field of permanent magnets, there is growing interest in additive manufacturing techniques and, in terms of materials, in recycling rare earth elements. In collaborative projects (Magneco CPP2023-010653, Llabor-0005) between the university and industry, permanent magnets have been synthesized using stereolithography or pellet extrusion. Additive manufacturing techniques favor the efficient creation of complex components, reducing costs and production times, improving quality, and allowing greater customization in diverse industries such as aerospace, the automotive industry, and renewable energy. In the industrial field, the creation/generation of optimized and sustainable designs for permanent magnets is expected, reducing dependence on rare earth elements and recycling obsolete materials, as well as new sustainable and scalable manufacturing processes. It is a project in development in which the optimization of processes and materials shows the need for interaction between academia and companies, requiring the complete characterization (morphological, compositional, chemical, mechanical, thermal, magnetic) of both materials and components. One of the problems to be avoided is the oxidation of recycled powder particles, which makes their reconditioning necessary. Regarding the components, the achievement of sufficient densification and magnetic response (saturation magnetization, coercivity) is necessary. The influence of the controlled application of an external magnetic field (assisted magnetic field and additive manufacturing) is also analyzed during the manufacturing process.



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sciforum-119416: Mechanism and Analysis of Orange Peel Formation on Bent Thin-Walled Copper Tubes

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Thin-walled pure copper tubes, extensively used in high-heat-flux electronic devices due to their excellent thermal conductivity, often develop orange peel defects during bending processes. This study compares tube samples with and without orange peel defects by analyzing their macro-surface morphology and microstructural evolution before and after bending. The crystal plasticity finite element model (CPFEM) was developed to explore the correlation between crystallographic orientation and surface defects. Finally, a multi-scale model of the tube bending process was developed by integrating the macroscopic finite element method (FEM) with the visco-plastic self-consistent (VPSC) approach to simulate and analyze the formation of orange peel defects on the outer wall of the tube at the bending site. The results indicate that high-temperature sintering causes significant grain coarsening and pronounced recrystallization textures in the matrix. Samples exhibiting orange peel defects contain banded annealing twins with textures distinct from the matrix, characterized by low Schmid factors and poor plastic deformation compatibility. CPFEM simulations demonstrate that during uniaxial stretching, "soft-oriented" matrix grains experience negative displacement along the surface normal, forming depressions, whereas "hard-oriented" grains undergo positive displacement, generating protrusions. This mismatch in localized deformation results in the formation of the macroscopic orange peel morphology. Simultaneously, the VPSC simulation results reveal that the number of activated slip variants differs between tubes with and without orange peel defects. Tubes with defects exhibit fewer activated slip variants and experience greater resistance to deformation.



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sciforum-115862: Metallic and half-metallic properties of full Heusler alloy Co₂MnGa with antisite defects

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Heusler compounds are attracting tremendous attention due to their significant magnetoresistance, half-metallicity, and other properties which are used in spintronics, magneto-optical, memory devices, etc. [1]. We performed first-principal calculations for compound Co₂MnGa, taking into consideration antisite structural defects. Co₂MnGa without antisite defects was confirmed to be a topological Weyl compound. The exact electronic states at E_F are 1.8 st./eV/f.u. in the majority spin and 0.58 st./eV/f.u. in the minority spin. Hence, the spin polarization is 52%. The magnetic moments are 0.73 (Co) μ_B , 2.91 (Mn) μ_B and -0.15 (Ga) μ_B , and the total moment of Co₂MnGa is 4.22 μ_B , which is in good agreement with the experimentally reported moment of 4.05 μ_B , which corresponds to the accuracy of our theoretical calculation being as high as 96%, it was previously calculated to be between 3.07 and 4.21 μ_B [1]. For the Co1-Mn antisite defect, the magnetic moment decreases to 1.07 μ_B ; for the Co2-Ga replacement, the magnetic moment is 1.85 μ_B . However, for the Co2-Mn antisite replacement, the total magnetic moment reaches up to 5.89 μ_B . Thus, the antisite defects in Co₂MnGa result in different changes in the magnetic moments and metallic properties, following from the densities of electron states calculated in our study.

Elphick, K.; Frost, W.; Samiepour, M.; Kubota, T.; Takanashi, K.; Sukegawa, H.; Mitani, S.; Hirohata, A. Heusler alloys for spintronic devices: review on recent development and future perspectives. *STAM* 2021, 22, 1, 235–271. <https://doi.org/10.1080/14686996.2020.1812364>



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sciforum-109477: Modified Sol–Gel Synthesis of SiO₂ Nanoparticles

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In this study, we successfully synthesized silicon nano-dioxide by modifying the conventional sol–gel method, eliminating the use of water as a hydrolysis agent and using oxalic acid as a reagent and structural reaction agent. The analytical results reveal that the product has a high purity and a coherent molecular structure. X-ray diffraction (XRD) analysis revealed a broad peak with an angle of 22.5°, indicating the morphosyntactic structure. Fourier transform infrared spectroscopy (FTIR) confirmed the presence of silicon dioxide bonds, while atomic force microscopy (AFM) revealed significant differences in surface morphology. In contrast to the typical spherical shape of silicon nano-dioxide, the surface of the synthesized silicon dioxide shows a mountainous terrain with marked peaks and valleys, with the distance between the lowest and highest points being less than 10 nanometers, indicating the small size of the nanocrystals. Ultraviolet (UV) spectroscopy revealed a distinct peak at a wavelength of 266 nm, corresponding to a small energy gap of 3.8 electron volts. This result shows that the synthesized solid has a semi-conductive character, unlike conventional silicon oxides, which are characterized by their insulating properties. Additionally, the unique morphology of the synthesized silicon dioxide nanoparticles suggests potential applications in various fields such as electronics, photonics, and catalysis. The modified sol–gel method employed in this study offers a novel approach to synthesizing silicon dioxide nanoparticles with tailored properties, paving the way for future research and development in nanotechnology.



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sciforum-114708: Ultrasonic Powder Atomization of Raney Nickel-type Precursors for Hydrogen Cathodes in Water Electrolysis

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Hydrogen, as an emission-neutral energy carrier, plays a key role in establishing a circular energy system and holds the potential to decarbonize numerous technical sectors. However, most hydrogen production to date has been derived from fossil fuels such as gray hydrogen. In contrast, sustainable green hydrogen can be generated by water electrolysis using renewable electrical energy. Yet, this remains economically unviable due to the comparatively low efficiency and high costs of precious cathode materials such as platinum. Hence, Raney nickel-type cathodes present a cost-efficient alternative due to their catalytic material properties. In perspective, thermally sprayed precursors are promising thanks to their characteristic open-porous structure, which is beneficial in applications such as atmospheric plasma spraying. Subsequent leaching of aluminum-rich phases chemically activates the surface and a nickel structure with a high specific surface area remains, which will enhance cathode reactivity. Prior to spraying, however, an appropriate powder feedstock must be identified. Also, the production by powder atomization is to be evaluated in order to meet the requirements for the indented application, including chemical homogeneity and composition, powder morphology and microstructure, phase formation, as well as particle size distribution. Therefore, in this study, preselected metal wires were arc-melted to rods with various compositions and subsequently ultrasonically atomized. Furthermore, bulk specimens were produced by spark-plasma sintering with low oxidation and low porosity. The material properties were examined along this process chain and related to the required functional properties, providing a comprehensive assessment of this approach.



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Session 6. Additive Manufacturing

sciforum-115954: Friction stir welding of laser powder bed fusion additively manufactured aluminum and copper alloys

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This study examines the feasibility of using friction stir welding (FSW) to join laser powder bed fusion (LPBF) additively manufactured Scalmalloy®, A20X, and CuNiSiCr copper alloys. Additively manufactured aluminum and copper alloys are highly valued for their ability to produce complex geometries. However, challenges such as printability issues, defect management, and the limited production volumes achievable with standard LPBF machines contribute to hindering their large-scale adoption. Consequently, researchers are increasingly exploring welding techniques for joining additively manufactured components. While fusion welding introduces challenges related to melting and solidification, solid-state welding methods like FSW offer significant advantages by preserving the engineered microstructures of these materials.

This research investigates the effects of FSW on the quality of butt joints made from 4 mm thick LPBF-manufactured plates of A20X, Scalmalloy®, and CuNiSiCr. A range of rotational and welding speeds was tested to evaluate the influence of the joining process on the mechanical properties and microstructures of these alloys. For the aluminum alloys, FSW produced welds with refined microstructures and only minimal reductions in mechanical strength compared to the base material. In contrast, the CuNiSiCr alloy demonstrated an increase in strength after welding, attributed to the fine-grained microstructure in the stir zone compared to the coarse-grained base material. Furthermore, 3D X-ray computed tomography revealed that metal stirring during the FSW process significantly reduced the intrinsic porosity across all the tested alloys. The study also evaluated hardness profiles, joint appearance, and fractographic analyses, highlighting a strong correlation between microstructural features and mechanical performance. These findings underscore the potential of FSW as an effective joining method for LPBF-manufactured components.



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sciforum-114978: Development of new stainless steel via Laser powder bed fusion process

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Laser Powder Bed Fusion (L-PBF) is one of the most important metal additive manufacturing (AM) methods, with various applications in industries such as the medical and automotive sectors, where precision and customization are essential. This research emphasizes integrating machine learning (ML) techniques with experimental analyses to optimize L-PBF processes. It provides critical insights into the interplay among process parameters, microstructure, and mechanical performance. This study employs ML to model the relationship between process parameters and relative density in AISI 316L stainless steel components containing 2.5% copper, produced via L-PBF. Support Vector Regression (SVR) was identified as the most precise algorithm for predicting relative density, with an accuracy of over 99%, enabling the optimization of process parameters to achieve desired outcomes such as high density, improved surface quality, or enhanced productivity. Subsequently, microstructural and mechanical properties were analyzed to provide deeper insights into material behavior. Microstructural investigations using Scanning Electron Microscopy (SEM) and Optical Microscopy (OM) revealed substantial transformations, including forming equiaxed and columnar cells attributed to copper addition. Irregular grains were observed, resulting from the rapid solidification characteristic of the L-PBF process. Notably, copper fully dissolved into the austenitic phase with no evidence of segregation, leading to increased lattice distortion, reduced crystallite size, and enhanced hardness. Melt pool dimensions were analyzed across samples with varying process parameters, establishing correlations with porosity levels and microstructural refinement. Additionally, in-situ alloying with copper was found to improve mechanical properties slightly. Tensile testing further explored the relationship between porosity and mechanical properties, providing a comprehensive understanding of the impact of process parameters and material composition on overall performance. SEM analysis of the fracture surfaces identified both brittle and ductile failure mechanisms. Brittle fractures exhibited quasi-cleavage planes, likely aligning with melt pool boundaries, while ductile fractures displayed extensive dimple networks.



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sciforum-114976: Machine learning-assisted material development via Laser powder bed fusion process

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Metal additive manufacturing (AM) revolutionized the fabrication of complex metal components, providing remarkable precision and flexibility in producing complex geometries. Integrating artificial intelligence (AI) can further revolutionize this field by highlighting complex relationships within manufacturing systems and enhancing quality control. Machine learning (ML) methods provide innovative solutions to optimize resource consumption, improve process efficiency, and address manufacturing challenges by correlating process parameters, material properties, part geometry, microstructural characteristics, and their resultant properties. In metal AM processes, ML applications extend beyond process optimization to include defect detection, in situ monitoring, and the enhancement of manufacturability and repeatability of components. This study optimizes key process parameters in laser powder bed fusion (L-PBF) to correlate the processing parameters and defect content in AISI 316L-2.5%Cu components. By applying ML algorithms, this research identifies optimal process parameter combinations to achieve specific objectives such as high production rate, low defect content, or superior surface quality. Seven ML algorithms (Bayesian Regression, Decision Tree Regression, Gradient Boosting Regression, Gaussian Process Regression, K-Nearest Neighbors Regression, Random Forest Regression, and Support Vector Regression) were systematically evaluated for their predictive accuracy across varying training and testing dataset sizes. Support Vector Regression (SVR) with a training size of 80% was chosen as the most accurate model for relative density prediction, with an average error of 0.62%. The optimized process parameters, derived from the best-performing ML model prediction, demonstrated a precise relationship between process parameters and defect content for achieving relative density values above 99.5% or high productivity. The optimized parameters obtained from this approach highlight the potential of ML-driven methodologies to balance productivity and defect content in AM processes. These findings demonstrate the importance of ML in advancing L-PBF technology and its broader applicability in metal AM.



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sciforum-094928: Electroless Nickel plating of Microglass balloons (MGBs)

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This study presents a thorough exploration of borosilicate microglass balloons (MGBs) with a focus on their potential application in aerospace engineering. The research encompasses the preparation, characterization, and modification of MGBs utilizing advanced techniques aimed at enhancing their functionality and performance within aerospace composite materials. Initial efforts involved the synthesis of MGBs according to established protocols, followed by meticulous characterization employing Scanning Electron Microscopy (SEM) and Energy Dispersive X-ray Spectroscopy (EDS). SEM analysis provided insights into the particle size distribution, with a particular emphasis on the AlSi10Mg alloy, revealing an average size of 35 μm . Concurrent EDS examination confirmed the elemental composition of the alloy. Subsequent utilization of MGBs as reinforcement within the AlSi10Mg matrix revealed an average particle size of 75 μm , with EDS analysis identifying key constituent elements, including Si, O, Na, Ca, and Au. To further enhance the properties of MGBs, systematic surface treatments were conducted under varying chemical compositions and temperatures, guided by Taguchi methods. Post-treatment SEM analysis demonstrated a notable reduction in average particle size to 60 μm , corroborated by EDS analysis of the altered chemical makeup. Fourier Transform Infrared (FTIR) spectroscopy provided valuable insights into the formation of essential chemical bonds, particularly C-C and C-O bonds, indicative of improved covalent bonding and mechanical properties. Additionally, activation treatments were implemented to introduce functional groups onto the MGB surface, as confirmed by SEM analysis, revealing a particle size distribution averaging 75 μm . EDS analysis further detected the presence of catalytic elements such as Cu, Ag, and Bi, contributing to enhanced layer adhesion. FTIR analysis confirmed the establishment of crucial C-O and CH₃ bonds, significantly augmenting surface wettability and adhesion properties.



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sciforum-113176: Material Anisotropy of non-heat-treated Inconel 718 Additively Manufactured by Wire Arc Additive Manufacturing

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Material anisotropy is an important topic to consider when using additive manufacturing for industrial applications. Since the products fabricated by wire arc additive manufacturing (WAAM), a metal additive manufacturing technology used to fabricate large parts, are sometimes used in parts that require a specific level of strength required by industry, it is essential to clarify the characteristics of these products for their industrial application. Furthermore, it should be noted that the fabrication of complex shapes such as blades by WAAM cannot be used for industrial applications, because of defective fabrication if appropriate fabrication conditions are not used. However, many studies have focused on simple shapes such as flat plates; thus, there is a problem in that evaluations have not always been conducted under conditions that enable the fabrication of complex shapes. In this study, an investigation was conducted into the material anisotropy of Inconel 718 under conditions where impeller blades can be fabricated by WAAM. An Inconel 718 wall was fabricated by WAAM, and tensile specimens were cut from the wall. Two different directions were used for the cutout: vertical and horizontal. Tensile tests were performed using these two types of specimens with different cutout directions. A comparison of the tensile test results showed that the difference between tensile strength and elongation at break was less than 3%. This indicates that the material anisotropy of Inconel 718 without heat treatment is small compared to other materials additionally produced by WAAM.



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sciforum-113164: Mechanical Properties of SST316L and Inconel 718 Multi-Material Additively Fabricated by Wire Arc Additive Manufacturing with Heat Treatment

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One approach to improving the manufacturing technology of turbomachinery is the application of metal additive manufacturing. Several studies have shown that wire arc additive manufacturing (WAAM) can be used to improve fabrication and reduce the environmental impact of impellers and other components with blades. To further advance manufacturing technology using WAAM, it is necessary to evaluate not only additive manufacturing using a single material, but also additive manufacturing combining multiple materials. However, there are only a limited number of examples of such studies. Therefore, there is a problem in that sufficient knowledge for industrial applications has not yet been obtained. The objective of this study is to evaluate the mechanical properties of a multi-material, stainless steel SST316L and nickel-based alloy, Inconel 718, fabricated by WAAM, when applied with heat treatment. To fabricate the test piece, a wall combining the two materials was fabricated by additively manufacturing an Inconel 718 wall made via WAAM and then additively manufacturing a SST316L wall on top of the Inconel 718 wall made via WAAM. A test piece was obtained by cutting out tensile test specimens from the wall. The specimens were subjected to several types of heat treatments and tensile tests were performed to analyze differences in their mechanical properties. The heat treatments were solution heat treatment, which is generally used for austenitic stainless steels, and aging treatment, which is generally used for Inconel 718. As a result, it was found that the multi-material under any of the heat treatments has mechanical properties that can be concluded to be industrially applicable.



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sciforum-114273: Optimization of Laser Powder Bed Fusion Parameters for Scalmalloy: Enhancing Print Quality and Mechanical Performance for Space Electronic Packaging

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Scalmalloy, an aluminum–magnesium–scandium alloy, is renowned for its exceptional strength-to-weight ratio and high ductility, making it a prime candidate for aerospace and space applications. This study focuses on optimizing the Laser Powder Bed Fusion (L-PBF) process parameters to enhance the print quality and mechanical properties of Scalmalloy components tailored for space electronic packaging applications where precise complex wall geometries and shape stability are crucial.

Employing Design of Experiments methodologies, we systematically varied key process parameters, including layer height, laser power, scanning speed, and hatch spacing. Standardized cubic specimens were fabricated across a range of energy densities to establish correlations between process parameters, porosity levels, and mechanical strength. Comprehensive analyses were conducted to evaluate the performance of these specimens. Our findings indicate that an optimal energy density window of 90 to 125 J·mm⁻³ minimizes porosity while maximizing mechanical performance.

Utilizing these optimized parameters, we designed and developed prototype components intended for space applications, emphasizing lightweight structures, thermal stability, and structural integrity. The results demonstrate that precise control of L-PBF parameters facilitates the production of Scalmalloy parts with superior mechanical properties and minimal defects, aligning with the stringent requirements of space applications. This research underscores the significance of parameter optimization in additive manufacturing to achieve resource-efficient production of high-performance metallic components.



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sciforum-113981: Performance Analysis of Ni-Doped SS316L Electro-Catalysts Synthesized via Wire Arc Additive Manufacturing (WAAM)

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India aims to produce five million tonnes of green hydrogen annually by 2030, which has ignited significant research into developing efficient and cost-effective production methods. Electrolysis, a critical environmentally friendly method for producing green hydrogen, faces challenges due to its reliance on costly precious metal electrodes, making it both expensive and inefficient. To reduce hydrogen production costs, this study investigates using wire arc additive manufacturing (WAAM) to create a Ni-induced Fe-Ni bimetallic structure (BS) as a cost-effective, alternative, and sustainable catalyst for efficient green hydrogen production. WAAM is an emerging technique that enables the deposition of multiple materials, such as stainless steel (SS) and nickel (Ni), layer by layer to create a BS with tailored properties.

The research focuses on the design and optimization of a BS by depositing different compositions of Ni (10% to 40%) in SS316L. The mechanical, metallurgical, and corrosion properties with oxygen evolution reaction (OER) activities were evaluated using corrosion, electrolysis, X-ray diffraction, and scanning electron microscopy.

This study revealed that increasing Ni content reduces micro-hardness by up to 38.14% due to higher L10-FCC phase formation. Similarly, increasing Ni content reduced the OER and corrosion activity, except for the 40% Ni content sample due to intermetallic formation (IMC) and lower polarization resistance. Further quenching heat treatment of the 40% Ni sample exhibited more remarkable performance than all other samples.

Finally, we have come to understand the effectiveness of WAAM in fabricating Ni-doped SS316L electrodes in an affordable way. IMC formation enhanced the activity of 40% Ni, and heat treatment plays a critical role in OER performance. Future work will explore other composition variations to understand the electrochemical behavior further, aiming to develop a scalable, cost-effective method for manufacturing green hydrogen-energy fuel-cell electrodes.



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Session 7. Corrosion, Wear, and Protection

sciforum-090990: Exploring the Influence of Polymer Additives on the Structure and Morphology of Copper Electrodeposits in Acid Sulfate Electrolytes

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This study conducted an exploration of the influence exerted by polymer ANP at various concentrations on Cu electrodeposition onto brass surfaces. This endeavor sought to illuminate the effects of the ANP additive while meticulously scrutinizing the morphology of Cu electrodeposits. To achieve this, a multifaceted approach was adopted, integrating techniques such as scanning electron microscopy (SEM) coupled with energy-dispersive X-ray spectroscopy (EDS) and atomic force microscopy (AFM). Cyclic voltammetry served as a pivotal tool in unraveling the Cu electrodeposition mechanism, unraveling an irreversible system characterized by diffusion-controlled kinetics. The SEM/EDS and AFM analyses unveiled compelling insights, showcasing that the incorporation of ANP resulted in an enhancement in the quality of Cu electrodeposits. This enhancement was notably reflected in the improved roughness and crystallite size of the deposits. Moreover, electrochemical measurements were conducted to probe ANP's influence on the resistance of Cu electrodeposits within a 3.5 wt% NaCl medium. These measurements brought to light a significant increase in the polarization resistance of the Cu deposit in the presence of ANP. This elevation underscored the heightened corrosion resistance conferred by ANP, particularly in marine environments notorious for their corrosive nature. The incorporation of ANP into the electrodeposition process heralded noteworthy advancements in both the quality and resilience of Cu electrodeposits. The enhanced morphology and increased resistance to corrosion observed in the presence of ANP underscored its potential as a beneficial additive in the realm of materials science, particularly for applications demanding durability in challenging environments like marine settings.



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sciforum-118392: PMMA–Siloxane–Silica Coating to Enhance Corrosion Resistance of AZ31

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Several studies in biomedicine have demonstrated the advantages of biodegradable and biocompatible metals for temporary implants, as they naturally degrade within the body, eliminating the need for surgical removal. Among them, magnesium–aluminium–zinc alloys, such as AZ31, show potential for controlled degradation in physiological environments, but their primary limitation is their rapid degradation.[1] This accelerated corrosion compromises implant integrity, leading to premature failure and limiting clinical applications. Thus, effective protective strategies are essential to enhance their corrosion resistance.

This study aimed to (a) perform a surface pretreatment to improve adhesion between the protective coating and the AZ31 alloy, and (b) develop a PMMA–siloxane–silica coating to reduce degradation. The formulation, based on 3-(methacryloyloxy)propyl trimethoxysilane and methyl methacrylate, was optimized for enhanced protective properties[2]. Its synthesis was characterized using real-time Fourier transform infrared spectroscopy, while its surface morphology and composition were analyzed via scanning electron microscopy and energy-dispersive spectroscopy. Corrosion resistance was evaluated through immersion tests in simulated body fluid (SBF) using potentiodynamic polarization and electrochemical impedance spectroscopy. Additionally, degradation behaviour was evaluated by monitoring pH variations and hydrogen evolution in SBF over time.

The results confirm that the PMMA–siloxane–silica coating significantly enhanced AZ31 corrosion resistance, ensuring controlled degradation. These findings present the potential of siloxane–silica coatings for biomedical applications.

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sciforum-114723: Wear and corrosion properties of SLM-manufactured 17-4PH components: Comparison of the effects of solution heat treatment, aging, and combined treatments

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Selective laser melting (SLM) has emerged as a versatile manufacturing method for complex metal components, offering high material utilization. 17-4PH stainless steel, which is known for its high strength and excellent corrosion resistance, is widely used in aerospace, biomedical, and mechanical manufacturing fields. However, the SLM process often results in microstructural features such as porosity and solute segregation, which significantly impact the wear and corrosion resistance of the produced components. Existing studies have primarily focused on the combined "solution heat treatment + aging" process, with limited research on individual solution or aging treatments. Furthermore, comparative studies on the effects of different heat treatment methods on wear and corrosion resistance remain insufficient. This study investigates the effects of three heat treatment methods—solution heat treatment (ST, 1 hour at 1040°C), aging treatment (AG, 1 hour at 480°C), and combined treatment (ST+AG, 1 hour at 1040°C followed by 1 hour at 480°C)—on the hardness, wear resistance, and corrosion resistance of SLM-manufactured 17-4PH stainless steel. The results reveal that aging treatment alone significantly enhances hardness, wear resistance, and corrosion resistance by optimizing the microstructure. Solution heat treatment improves microstructural uniformity and corrosion resistance but reduces wear resistance due to the complete transformation to a predominantly BCC structure. Combined treatment increases hardness but decreases wear and corrosion resistance due to precipitate formation. This study highlights the potential of aging treatment alone to enhance the performance of SLM-manufactured 17-4PH stainless steel, providing valuable experimental evidence for optimizing heat treatment strategies.



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sciforum-115190: Corrosion Behavior of Biodegradable Mg-Zn-Ca Alloy under Simulated Severe Post-implantation Inflammatory Conditions

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Magnesium alloys are promising candidates for temporary implant materials due to their biocompatibility, biodegradability, and ability to support tissue regeneration while gradually dissolving in physiological environments. However, the inflammatory environment near implants, characterized by the presence of reactive species and acidic conditions, can significantly influence their corrosion behavior. This study investigates the electrochemical corrosion performance of Mg-2.1wt% Zn-0.6wt% Ca alloy in three simulated physiological conditions: (1) normal medium (phosphate-buffered saline, pH 7), (2) inflammatory medium (PBS with H₂O₂ and HCl, pH 5), and (3) severe inflammatory medium (PBS with H₂O₂, HCl, bovine serum albumin [BSA], and lactic acid, pH 3).

Electrochemical tests, including potentiodynamic polarization and electrochemical impedance spectroscopy, were employed to systematically evaluate the corrosion rates and underlying mechanisms of the alloy in the three simulated media. The results demonstrated that the presence of H₂O₂ and an acidic pH significantly accelerated the corrosion rate of the Mg-Zn-Ca alloy, owing to the oxidative stress induced by H₂O₂, which promoted the formation of reactive oxygen species (ROS) that destabilized the magnesium hydroxide protective layer. The acidic pH further exacerbated the corrosion by dissolving the passivating Mg(OH)₂ layer, exposing fresh magnesium to the corrosive medium.

In addition, the inclusion of BSA and lactic acid in the severe inflammatory medium amplified the corrosion process. BSA, a protein that simulates the role of extracellular proteins, binds to the alloy surface and alters the local electrochemical environment by forming complexes with magnesium ions. This chelation effect destabilizes the surface and promotes ion release. Similarly, lactic acid, a byproduct of cellular metabolism during inflammation, acts as a weak organic acid that enhances the dissolution of magnesium hydroxide through acidification and ion chelation mechanisms. Together, BSA and lactic acid simulate conditions that reflect the inflammatory response and metabolic activity near implants, highlighting their synergistic impact on accelerating corrosion.



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sciforum-119354: Effect of Al content on corrosion behavior and mechanical properties of mold casting and high-pressure die casting Mg alloys

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The Al content plays a critical role in determining the corrosion and mechanical properties of AZ series Mg alloys. These properties have been widely investigated; however, the effects of high Al content above 9 wt.% on corrosion behavior, mechanical properties, and their relationship have not been explored. In this study, Mg-*x*Al-0.8Zn-0.1Mn-0.3Ca-0.2Y (*x*: 6, 9, 11, 13) alloys were prepared via mold casting (with a lower cooling rate) and high-pressure die casting (with a higher cooling rate) to investigate the effects of Al content on microstructure, corrosion behavior, and tensile properties. In particular, the tensile properties were evaluated before and after the salt spray test (SST). The corrosion rate was lower for the high-pressure die-casting alloy with a higher cooling rate than for the mold-casting alloy with a lower cooling rate. For mold-cast alloys, the corrosion rate increased significantly with increasing Al content. In contrast, for die-cast alloys, the corrosion rate initially increased and then decreased with higher Al content. The corrosion behavior was revealed to be related to the fraction and continuity of the β -Mg₁₇Al₁₂ phase and the Zn content within this phase through the EPMA and SKPFM analysis. Regarding mechanical properties, in both their initial state and their SST-exposed state, die-cast alloys exhibited improved strength with increasing Al content. Although the mechanical properties decreased after SST exposure, the extent of deterioration diminished with higher Al content.



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sciforum-119434: Functionalization of metal surfaces through plasma electrolytic oxidation (PEO) treatments with the addition of particles

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Plasma Electrolytic Oxidation treatment (PEO, which is sometimes also called MAO—Micro Arc Oxidation) has recently attracted a great deal of attention due to its ability to create a thick and adherent coating with excellent corrosion and wear resistance. Some of the main characteristics of PEO coatings are the high porosity of the outer layer and the possibility to incorporate directly into the coating particles that are dispersed into the electrolyte. In particular, this last characteristic is particularly useful due to the fact that it permits easy functionalization of the coated surface. The present work describes the results of the production and characterization of PEO-coated samples of aluminum and magnesium alloys obtained by inserting metallic and non-metallic particles into the coating. The coatings are produced with different current modes (direct or pulsed unipolar) and the incorporation occurs by simple dispersion of the particles into the electrolyte used for the PEO treatment. Several types of particles were inserted into the coatings: nano-particles of graphite were inserted in order to improve the wear resistance; metallic particles (copper or silver) were inserted in order to give to the samples bactericidal, fungicidal or antifouling properties; glass particles were included to improve the samples' wear and corrosion properties; and titanium dioxide particles were added to create photocatalytic surfaces. The obtained coatings were, in all cases, characterized both on the surface and in the cross-section through SEM analysis and X-Ray diffraction in order to confirm the presence of the particles and to study the microstructure and morphology of the obtained coatings. Later, specific tests were performed to confirm the specific functionality given to the surface (these took the form of corrosion tests, wear tests, biological tests, or photocatalytic tests). In all the cases, the results revealed significant incorporation of the particles into the coating and good specific functional properties.



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sciforum-119500: Integrated Molecular Approach for Assessing Microbial Corrosion Dynamics in Oil and Gas Infrastructure

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Microbially influenced corrosion (MIC) poses a significant threat to the oil and gas industry, leading to costly failures and disruptions across production, transportation, and storage systems. Traditional microbial assessment and mitigation strategies often rely on culture-based methods, potentially underestimating the complexity of corrosion-driving microbial communities. Here, we present an integrative methodology that combines third-generation sequencing technologies, quantitative polymerase chain reaction (qPCR), physicochemical analyses of operational environments, and 3D reconstructions of defects on metallic probes or coupons, complemented by a thorough examination of design and operational parameters. By targeting both planktonic and sessile bacterial populations, this approach enables a comprehensive evaluation of corrosion-inducing potential under site-specific conditions. Crucially, shifts in microbial community composition across diverse corrosive taxa provide early warnings of elevated corrosion risk, guiding adjustments to biocides, corrosion inhibitors, and failure analyses. This framework's inclusion of unculturable microorganisms underscores the importance of quantitative molecular methods in conjunction with or as an alternative to traditional culture-based techniques. Moreover, the integration of high-throughput sequencing data with advanced analytics supports the development of robust monitoring protocols, while the 3D mapping of metallic defects refines the detection of localized corrosion hotspots. By iteratively combining microbial profiling, defect reconstruction, and physicochemical parameters, this methodology refines monitoring strategies and defines key performance indicators (KPIs) that inform continuous optimization of corrosion management. Ultimately, this holistic and data-driven approach enhances the reliability and longevity of oil and gas infrastructure by enabling proactive, evidence-based decisions aimed at mitigating MIC effectively.



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sciforum-119389: Investigation of Surface Oxidation Behavior on High-Tensile Brass and its Effect on Hot Forging

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CW722R and CW617N brasses are well known for their good formability at elevated temperatures; hence, both alloys find application in forging applications. In practice, it has been observed that CW722R alloy requires a slightly higher forging temperature than CW617N. Studies on other alloys have shown that the response to manufacturing is related to the characteristics of the oxide formed in the surface. However, no studies have been performed to show the effect of surface oxidation on brass during forging. Therefore, the surface oxidation behavior of a CW722R and CW617N alloy was investigated during manufacturing, and its effect on forging was explored. For this purpose, SEM-EDS analysis was performed on the surface of the samples in order to measure the depth of the oxide layer and identify the composition of the oxide. In addition, thermodynamic and Pilling-Bedworth ratio calculations were employed to determine the chemical composition of the oxide layers and explain their mechanical response. The results show that the oxide layer consists of Cu₂O/ZnO/PbO with an average width of 0.81µm to 4.1µm according to SEM-EDS analysis and thermodynamic simulation. The Pilling-Bedworth ratio was assessed, showing that the oxide layer is cohesive and protects the surface from further oxidation. In addition, the oxide layer has lower thermal conductivity than the alloy; therefore, during hot forging, the lower thermal conductivity of oxide layer helps to maintain the temperature at higher degrees and thus reduces the forging load.



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sciforum-119497: Methodological Routes for Failure Analysis in Continuous Rods for Artificial Lift Systems: A Data-Driven and Damage Characteristic Approach

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One of the key components in the reciprocating lift system and progressive cavity pump system is the steel rod string. This part is in charge of two main objectives in oil production. First, it allows the transmission of movement from surface to downhole, and secondly, it permits fluid lift. Nowadays, the use of continuous rods instead of conventional coupling rod systems has gained considerable attention due to its advantages like the higher amount of annular space available for production, less complex installation, and better distribution of contact loads with tubing. Understanding the reasons for continuous rod failure important to improve the performance and propose improvements in its design, use, and materials. Herein, an extensive data analysis of 51 failures in continuous rods has been performed, providing principal insights to identify the damage mechanisms, and, through fractography analysis, the principal service loads are identified. All the analyzed failures have occurred due to fatigue, implying that fatigue design and assessment are necessary for successful rod performance. Stress concentrators have been caused due to abrasion related to sand management, friction between the tubing and the rod, corrosion (CO₂, microorganisms), issues with rod manufacture quality, operative conditions, installation, and synergies between them. Our results show that the three main reasons for failure are corrosion (31.4%), fretting corrosion (13.4%), and abrasion–corrosion (11.8%) which are related to service conditions, and their principal morphological features were identified. Also, manufacturing rod quality is the source of 9.8% of failures. This provides a useful guide for engineers to find an easy way to identify the reasons for failure in their oilfields. Finally, a comprehensive analysis of the principal used metallurgies is presented, presenting their main advantages, limitations, quality control benchmarks, and future perspectives for new materials in this component.



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sciforum-118763: Microbial corrosion in oil transportation and storage systems: laboratory-scale study on biofilm and pitting formation

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Microbiologically influenced corrosion (MIC) is critical in oil transportation systems, where biofilm formation accelerates metal deterioration, often leading to structural failures and economic losses. Several microbial groups contribute to MIC by interacting with the metal surface or by producing corrosive metabolites that facilitate localized metal loss. In this study, the microbial communities of pigging scrapings and water produced from crude oil and naphtha storage tanks in several oilfields in Colombia were characterized using next-generation sequencing technologies. Additionally, laboratory simulations evaluated MIC and biofilm formation under dynamic and static conditions using native microbial strains. Carbon steel coupons (AISI/SAE 1018) were installed in custom-designed bioreactors, a side-stream system, and exposure setups developed by the Corporación para la Investigación de la Corrosión (CIC). Exposure times ranged from 6 hours to 120 days. Sessile bacterial counts were performed with liquid culture media, complemented by microscopy (SEM) for biofilm characterization and pitting depth determination. Biofilm formation was detected within 12 hours, while sessile SRB colonization occurred at 6 hours. After 90 days, the localized MIC pitting reached 35.5 μm , with a maximum corrosion rate of 5.5 mpy, classified as moderate according to the standard AMPP SP 0775-2023. These findings highlight rapid biofilm development and its correlation with MIC severity under both dynamic and static conditions. The present analysis confirms that the microbial composition associated with production has significant corrosive potential. The presence of these microorganisms and the pitting depths observed indicate a clear MIC threat in such systems. Implementing routine microbiological monitoring, optimizing maintenance schedules, and strengthening internal pipeline cleaning procedures are recommended to reduce the threat of MIC. In the case that MIC materializes in field-installed biocoupons and coupons, biocide treatments should be considered to prevent further structural degradation of oil transportation and storage systems.



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sciforum-115102: Numerical simulation of galvanic corrosion of a tube-fitting steel assembly in a chloride environment

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Galvanic corrosion is a complex and significant issue that affects metal structures across various industrial environments, especially in the presence of chloride solutions. In this study, we investigate the galvanic corrosion behavior of a steel tube assembly exposed to a chloride solution using advanced numerical simulation software. By leveraging multiphysics modeling techniques, we developed a comprehensive numerical model that integrates the electrochemical processes involved in galvanic corrosion. This model considers the electrochemical properties of the materials comprising the assembly and the environmental conditions, such as chloride solution concentration and conductivity.

Our study focuses on key parameters including corrosion rate, corrosion potential, and the distribution of damage within the assembly. The simulation results reveal critical insights into the mechanisms governing galvanic corrosion, offering a deeper understanding of how these factors contribute to the degradation of metal structures in chloride-rich environments. Additionally, our findings enable the prediction of the long-term behavior and performance of such assemblies under corrosive conditions.

This numerical approach presents a cost-effective and efficient alternative to traditional experimental methods, facilitating the evaluation and optimization of corrosion protection strategies. By reducing reliance on extensive physical testing, our model supports the design and implementation of more effective corrosion mitigation measures, ultimately extending the lifespan and reliability of metal structures in challenging environments.



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sciforum-115159: Optimization of Zn-Ni Alloy coating to enhance corrosion resistance of carbon steel

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Zn-Ni alloys have gained considerable attention due to their superior ability to resist corrosion. Zn-Ni electroplating can be improved by optimizing the nickel composition in Zn-Ni alloys, which provides better protection compared to Zinc deposited alone; it can also be improved by incorporating additives into the plating bath. The aim of our research was to optimize our electroplating bath by adding an eco-friendly additive to enhance the characteristics of the deposits obtained, particularly their morphology after electrodeposition, and their resistance against corrosion, using different concentrations of this additive (0g/l, 0.25g/l, 0.5 g/l, 1g/l and 2g/l). Several deposits were made for this purpose and their properties were investigated. We used scanning electron microscopy (SEM) to examine the deposits' surface morphology, while energy-dispersive spectroscopy (EDS) was used to assess the chemical composition of the deposits. Electrochemical methods, polarization measurement (PDP) and electrochemical impedance spectroscopy (EIS), were used to investigate the corrosion resistance of every deposition in an ASTM D1384-87 medium. The results show that the incorporation of the eco-friendly additive into the electroplating bath significantly improves both the morphology and corrosion resistance of Zn-Ni coatings. Compared to all the deposits produced in this study, the optimum concentration is 1g/l of the additive, which produced the most corrosion-resistant Zn-Ni alloy deposit.



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sciforum-114784: Study of Crevice Corrosion in X70 pipeline Steel Using a 2D Finite Element Model

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X70 steel, a high-strength low-alloy (HSLA) steel, is extensively utilized in energy transport pipelines due to its exceptional mechanical properties, including robustness, ductility, and resistance to high-pressure environments. Despite these advantages, X70 steel is susceptible to crevice corrosion, a localized form of corrosion that occurs in confined spaces, such as overlaps, joints, or gaps. This type of corrosion can severely compromise the structural integrity and longevity of pipelines, leading to costly maintenance and safety concerns.

This study focuses on understanding the complex mechanisms underlying the crevice corrosion of X70 steel when exposed to a 0.3 M NaCl solution. A two-dimensional multi-physics finite element model was employed to simulate the corrosion process, providing valuable insights into the electrochemical phenomena involved.

The findings indicate a heterogeneous distribution of electrochemical potential within the crevice, accompanied by an exponential decrease in current density as the depth increases. This behavior is largely attributed to the ohmic drop (IR) effect. Additionally, geometric deformations were observed to progressively intensify, with the most severe damage occurring near the crevice opening. These results emphasize the need for improved designs and mitigation strategies to minimize the risks associated with crevice corrosion in X70 steel pipelines, thereby enhancing their safety, longevity, and durability in service.



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sciforum-114472: Synergistic applications of polypyrrole coatings in aluminum food cans: From corrosion protection to VOC sensing

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The increasing demand for advanced food packaging technologies has prompted the exploration of functional coatings that can extend the shelf life of food products while maintaining safety and quality. In this study, polypyrrole coatings were synthesized on aluminum can metals using various electroanalytical techniques across different electrolytic media, namely oxalic acid, sodium salicylate, and acetonitrile. The resulting films were subjected to extensive characterization through spectroscopic and microscopic techniques to assess their structural and compositional properties. The primary objective of this work was to evaluate the effectiveness of these polypyrrole (PPy) coatings in providing corrosion protection to aluminum cans, a critical factor for maintaining the integrity of food containers. Additionally, the films' ability to detect volatile organic compounds (VOCs) was investigated, aiming to incorporate sensory functionalities into the packaging system. The results demonstrated that the polypyrrole coatings significantly enhanced the corrosion resistance of aluminum in various aggressive environmental conditions. Moreover, the films exhibited promising sensitivity to VOCs, paving the way for the development of intelligent packaging systems capable of the real-time monitoring of food freshness. This research underscores the potential of polypyrrole-based coatings as multifunctional materials for smart food packaging applications, combining protective and sensory capabilities to improve food safety and quality.



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sciforum-119172: The effect of biocidal treatments on native thiosulfate-reducing bacteria that contribute to biocorrosion in the oil and gas sectors

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Microbiologically influenced corrosion (MIC) is a phenomenon that contributes to the deterioration of metallic materials in industrial environments. This process has a significant impact on the infrastructure of oilfields, primarily affecting pipelines, storage tanks, and water distribution systems. The main bacterial groups associated with biocorrosion can be classified based on the metabolic pathways they employ. These include sulfate-reducing bacteria (SRB), acid-producing bacteria (APB), and thiosulfate-reducing bacteria (TRB), among others, which colonize and degrade metal surfaces through various metabolic mechanisms. This study aimed to evaluate the efficacy of different biocidal compounds in controlling TRB under laboratory conditions. The modified Time Kill Test (TKT) technique was employed using special BioCIC liquid culture media from the Corporación para la Investigación de la Corrosión (CIC). Seven biocide treatments were tested, including formulations based on tetrakis (hydroxymethyl) phosphonium sulfate (THPS), quaternary ammonium, and glutaraldehyde, among others. Bacterial incubation was conducted at 70°C for 28 days to simulate field conditions. To identify microorganisms associated with biocorrosion in the production water at a Colombian oilfield, total genomic DNA was extracted from the samples and sequenced using the Oxford Nanopore Technology. Among the tested treatments, the M1 formulation (quaternary ammonium 10–30%, THPS 10–30%, and glutaraldehyde 10–30%) exhibited the highest antimicrobial efficacy, significantly reducing bacterial growth compared to the other biocides. The molecular identification of microbial communities in production water samples from seven different field locations revealed *Thermotoga* and *Thermovirga* as the predominant genera. However, post-TKT cultures treated with M1 showed a shift in microbial composition, with *Acetomicrobium* emerging as the dominant genus. These findings highlight the importance of evaluating diverse biocidal formulations to optimize MIC control strategies. Additionally, characterizing microbial populations in production waters is crucial for developing targeted mitigation approaches tailored to the specific microbial consortia present in each field.



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Session 8. Metallic Materials Processing

sciforum-112145: Effect of synergistic burnishing–tumbling treatment on surface roughness, microstructure, hardness and mechanical strength of AISI 304 alloys

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Any metal component failures (e.g., corrosion, fatigue) start from surface/subsurface defects (e.g., surface cracks, troughs, and pores). It is thus crucial to strengthen surface integrity by altering surface/subsurface properties in ways which provide protection from premature failure. To address this, in this paper, we presented a synergistic plasticity burnishing plus tumbling treatment to enhance the surface integrity and mechanical properties of cold-rolled AISI 304 steel alloys. A total of 304 steel specimens were ball-burnished, followed by a rotary tumbling process. The treated specimens were characterised in terms of surface roughness, 2D/3D topography hardness, and microstructures using laser confocal microscopy, SEM, a micro-hardness tester and EBSD analysis, respectively. Tensile tests were performed in accordance with ASTM standards to evaluate the Young's modulus, yield strength, UTS and elongation. To evaluate the efficacy of the proposed synergistic approach, the results were compared and analysed across four types of specimens referred to as (1) "Untreated (as rolled)", (2) "Burnished", (3) "Tumbled" and (4) "Burnished+Tumbled". The results showed that the ball burnishing resulted in grain modification and dislocation within the microstructure, improving the hardness and surface finish. But when the tumbling was applied to the burnished surface, the process augmented further hardness, grain modification, and yield strength, while there was a negligible impact on the fracture strength and elongation. These improved surface integrity properties are expected to enhance corrosion and fatigue life. The findings indicate that the combined burnishing–tumbling approach can extend the operational life of components subject to extreme loading conditions, thus saving huge costs by minimising premature failure.



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sciforum-115029: Laser marking of stainless steel and aluminum

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The marking of components using laser technology is a permanent process that utilizes a beam to create a mark, or even engrave, on the surface of a component. Based on the potential for a high marking quality, this process is increasingly employed across various industries (semiconductors, electronics, medical, automotive, aerospace, etc.) for engraving serial numbers, logos, barcodes, QR codes, and more. Several laser processing parameters influence the marking quality as well as penetration. Depending on the component and material involved, these parameters must be adjusted to determine the optimal settings for each component/material. This study investigates the influence of laser beam parameters on marking quality to achieve the best set of laser marking conditions for different metals. A 30 W fiber laser was utilized, and the parametric study focused on power, frequency, marking speed, and the number of passes. The materials studied included aluminum alloy AW-6082-T6 and stainless steel 304 2B. The results demonstrate that the markings varied in color and quality, and it was possible to identify the optimal parameter sets for each material to ensure the best marking quality, even at high marking speeds. Overall, the marking strategy also influenced the marking quality, including the presence or absence of contours and the fill method used. This investigation also identified the degradation mechanisms associated with each material and how to mitigate undesirable effects, ensuring that the markings comply with industrial standards.



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sciforum-118642: Exploring the Impact of MIG Brazing Techniques on Stability, Bead Morphology, and Joint Performance

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This study explores the influence of various Metal Inert Gas (MIG) brazing modes on critical factors such as the process stability, bead morphology, microstructure and mechanical performance of brazed lap joints of dual-phase (DP600) steel. Through systematic analysis of voltage/current signals and deposition characteristics, this research reveals how variations in heat input impact material flow and wettability during the brazing process. A higher heat input has been found to enhance wettability and improve joint strength, yet it can lead to a reduction in the cross-sectional area, ultimately affecting resistance to failure. Conversely, lower heat inputs contribute to more stable deposition, which enhances resistance to failure and defects, but too low wettability can also cause premature failure of the joints. Additionally, this study identifies key process behaviours, including the tendency for increased instability at higher wire feed rates and the significant role of bead morphology in determining mechanical performance. By elucidating these process–property relationships, this research provides a valuable framework for selecting appropriate MIG brazing parameters tailored to specific applications. The findings significantly contribute to the development of process control strategies aimed at enhancing joint reliability, offering critical insights for industries focused on optimizing brazing techniques to achieve improved structural integrity and overall performance in their applications.



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sciforum-114991: The Directional Solidification of Al-Zn Alloys as a function of the Level of Convective Heat Transfer

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In this study, an analysis of the directional solidification of Al-Zn alloys using a Bridgman-type rotary directional solidification device is presented. For this purpose, the device can be rotated at three tilt angles (0°, 90°, and 180°). Directional solidification tests were performed with Al and Zn (commercial grade) and with Al-5%Zn and Al-10%Zn alloys (weight percent). The aim is to analyze how the furnace inclination (which generates different levels of convective heat transfer in the solidifying specimen) and the alloy composition influence the cooling rate of the metallic solid, the thermal gradients, and the size of the macrostructure and microstructure present. It has been observed that by varying the furnace inclination angles, for the same composition, the cooling rate tends to decrease; it is also important to highlight that the minimum temperature gradients coincide with the position of the CET. For commercial purity Al, average cooling rates of 2.21 °C/s at 90°, 2.05 °C/s at 45°, and 1.98 °C/s at 0° were obtained for each of the tests. For the Al-10wt. %Zn alloy, average cooling rates of 2.43 °C/s at 90°, 2.14 °C/s at 45°, and 1.99 °C/s at 0° are obtained, with a clear decrease in the cooling rate as the furnace tilt angle is varied. Similarly, when the CET occurs, the critical gradient value is -0.5 °C/cm for Al, 0.1 °C/cm for Zn, 1.4 °C/cm for Al-5wt. %Zn, and -1.2 °C/cm for Al-10wt. %Zn. On the other hand, when analyzing the behavior of Zn, it can be highlighted that the cooling rate values decrease significantly when compared with Al (both commercial grades) and with the Al-5wt. %Zn and Al-10wt. %Zn alloys. These data indicate that the alloy composition and the inclination of the solidification device influence the cooling rate and the thermal gradients.



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sciforum-114819: The Potential Property-Tailoring Effects of Cryogenic Treatment on Pure Zinc

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As of late, there has been increasing scope and demand for implants in the biomedical sector, notably in the field of orthopaedics. Within this field, zinc (Zn) is a promising base metal for such implants due to its combination of biocompatibility, mechanical properties, and corrosion response.

For the first time, pure Zn was successfully synthesized using the Disintegrated Melt Deposition (DMD) method and subjected to systematic cryogenic treatment (CT) study, with exposure to varying subzero temperatures ($-20\text{ }^{\circ}\text{C}$, $-50\text{ }^{\circ}\text{C}$, $-80\text{ }^{\circ}\text{C}$, and $-196\text{ }^{\circ}\text{C}$) for a duration of 24 hours. Densification occurred for all materials (with a 35.9% porosity reduction after exposure to $-50\text{ }^{\circ}\text{C}$ being the most significant). Microstructurally, CT induced significant grain growth across all exposure temperatures, with $-80\text{ }^{\circ}\text{C}$ conferring the largest grain size (224% increase over as-extruded equivalent). The compression response was also improved slightly after exposure to $-50\text{ }^{\circ}\text{C}$, with improvements of 2.7%, 2.3%, and 1.0% to compressive yield strength, ultimate compressive strength, and work of fracture, respectively. Exposure to $-196\text{ }^{\circ}\text{C}$ also notably lowered corrosion rates (32.4% reduction compared to as-extruded equivalent).

These findings highlight the ability of CT to not just alter but tailor the individual properties of Zn-based materials, useful in specific applications. Furthermore, this also opens up a new research area for this Hexagonal Closed Pack (HCP) metal and its derivatives.



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Session 9. Metallic Materials for Biomedical Applications

sciforum-115059: A review on perovskite magnetic nanoparticles (MNPs) used in magnetic hyperthermia (HT)

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Magnetic hyperthermia (MHT) has emerged as an innovative cancer treatment modality that involves the generation of heat by exposing magnetic nanoparticles (MNPs) to an alternating magnetic field (AMF). This approach has attracted considerable attention due to its ability to locally elevate the temperature of tumor tissues in a non-invasive manner. MHT can be used either as a standalone treatment or in combination with other therapeutic strategies, such as surgery, chemotherapy, or radiotherapy, enhancing the overall therapeutic outcome. Among the various magnetic materials available for hyperthermia applications, perovskites stand out due to their unique crystalline structure and versatile electronic and magnetic properties. These characteristics make perovskites promising candidates for developing highly efficient MNPs that can be fine-tuned to optimize heat generation under an AMF.

This review focuses on the magnetic properties of perovskite-based nanoparticles and their potential for use in MHT. The article discusses several perovskites that have been explored for hyperthermic applications, examining their structural, magnetic, and thermal properties. Additionally, the synthesis methods employed for fabricating perovskite-based MNPs are thoroughly reviewed. Despite the promising potential, challenges remain in harnessing the full capability of perovskites in MHT, including issues related to stability, biocompatibility, and scalability. These limitations are also addressed in this review, and future directions are proposed, ensuring the widespread adoption of perovskites as efficient and reliable MNPs for magnetic hyperthermia in clinical settings.



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sciforum-115015: Creation of thin TiNi wires with stabilized martensite phase

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TiNi-based alloys have a unique set of functional and structural properties, which allows them to be used as materials for creating implants. Thin TiNi threads were obtained by drawing with intermediate chemical and mechanical treatments. Thinning the threads to 40-60 μm made it possible to manufacture textile implants for use in soft tissues of the human body. However, the Young's modulus (E) of metallic TiNi-based materials can exceed that of soft connective tissues. Cryogenic treatment can reduce the elastic modulus by stabilizing the martensite phase and thereby reducing the rigidity of the material. This approach is novel and helps solve a fundamental problem in medical materials science.

Thin TiNi wires were obtained through the traditional technique and cryogen treatment. X-ray diffractometry, scanning electron microscopy, and energy dispersive spectroscopy allowed for determination of the structure and phase composition of thin wires with a composite structure based on TiNi(B2), TiNi3, TiC, and TiO2 phases. It was shown that the cryogenic treatment of thin TiNi wire resulted in the formation of two phases B2+B19 in the structure, which indicated martensite stabilization after cooling. The porosity of the obtained implants was 80 to 85%. SEM images of the structure of spherical implants after biointegration show the high integration tie between these implants and animal tissues. The high integration tie was observed between body tissues both inside and on the surface of the spherical implant.

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sciforum-115106: Development of Mg-1Zn-1Ca-xZnO (x = 0 and 2 wt.%) composite using disintegrated melt deposition method for biomedical applications

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Magnesium (Mg)-based biodegradable materials have become prominent for use in temporary implant applications. In the present work, the Mg-1Zn-1Ca-xZnO (x = 0 and 2 wt. %) alloy and composite were synthesized using a disintegrated melt deposition (DMD) technique followed by a hot extrusion process, and their microstructure, thermal, and mechanical properties were studied. The average grain size for the Mg-1Zn-1Ca alloy and the Mg-1Zn-1Ca-2ZnO composite obtained is 7.0 μm and 6.3 μm , respectively. The XRD analysis depicted that 10-11 pyramidal planes are dominant, and Mg_2Ca , Mg_2Ca and MgZn phases are formed in the Mg-1Zn-1Ca alloy and the Mg-1Zn-1Ca-2ZnO composite. The modulus of elasticity increased by 3.30 % and the ignition temperature increased by 3.11 % with the addition of 2 wt. % ZnO nanoparticles in the Mg-1Zn-1Ca alloy. The Vickers hardness value increased by 1.70 % while the yield strength increased by 13.77 % after the addition of ZnO nanoparticles (150.3 MPa and 171.0 MPa, respectively, for the monolithic Mg-1Zn-1Ca alloy and Mg-1Zn-1Ca-2ZnO composite materials, both of which exceed the yield strength of natural bone at 60 - 90 MPa). The results demonstrate the efficacy of ZnO nanoparticles for use in biomedical applications with good mechanical properties.



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sciforum-115216: Enhanced Corrosion Resistance of Ti-6Al-4V Alloys via SLA-Treated Alginate-Based Hydrogels Incorporating CuO Nanoparticles

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The biocompatibility and durability of titanium alloys, such as Ti-6Al-4V, are critical for their performance in biomedical applications. However, their susceptibility to corrosion in physiological environments remains a challenge. This study explores the synthesis and application of alginate-based hydrogels loaded with copper oxide nanoparticles (CuO NPs) as a protective coating on untreated and SLA-treated Ti-6Al-4V substrates. Alginate, a biopolymer with high hydrophilicity and biocompatibility, was selected for its potential to create a uniform hydrogel layer, while CuO NPs were incorporated for their known antimicrobial and corrosion-inhibitory properties. SLA treatment was employed to enhance surface roughness, promoting hydrogel adhesion.

The synthesized hydrogels were characterized using FTIR, confirming the successful incorporation of CuO NPs. Adhesion testing demonstrated superior hydrogel attachment to SLA-treated titanium surfaces due to increased surface roughness and energy. Corrosion resistance was evaluated using potentiodynamic polarization and electrochemical impedance spectroscopy (EIS) in a simulated body fluid. The results revealed significant improvement in corrosion resistance for the hydrogel-coated samples compared to bare titanium, with the CuO NP-loaded hydrogels exhibiting the highest protection. This enhancement is attributed to the hydrogel's barrier properties, which limit ion diffusion and reduce electrolyte access to the metal surface, counteracting the expected corrosion-promoting effect of a wet environment.

This research highlights the potential of SLA-treated, CuO NP-enriched alginate hydrogels to improve the longevity and performance of titanium implants by addressing both biocompatibility and corrosion resistance challenges.



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sciforum-119623: Exploring the potential of nanostructured metals in biomedical applications: a review of their properties, challenges, and future directions

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Nanostructured metals have gained considerable attention in biomedicine due to their superior properties, including enhanced wear resistance, improved biocompatibility, and the ability to interact favorably with human tissues. These materials are highly suitable for applications in the development of bioactive implants, prosthetics, medical devices, and other areas requiring high-performance materials. Compared to traditional metals, nanostructured materials exhibit significantly improved mechanical and chemical behaviors, enhancing their integration into the human body and reducing the risk of rejection or complications post-surgery.

A key advantage of nanostructured metals in biomedicine is their ability to improve biocompatibility by manipulating grain size and structural features at the nanometer scale. This modification enables better interaction with human tissues, minimizing risks such as inflammation or adverse reactions. Furthermore, nanostructuring significantly boosts the mechanical properties of metals, such as tensile strength and durability, making them ideal for prosthetics and implants that must endure substantial mechanical stress over extended periods.

Additionally, nanostructured metals can create bioactive surfaces that promote tissue regeneration or enable the targeted delivery of therapeutic substances. These capabilities make them particularly promising for controlled drug release applications, such as releasing anti-inflammatory or antibiotic agents directly at the site of injury or infection, thereby improving recovery times and preventing post-operative complications.

Nanostructured metals hold great promise for biomedical applications, but challenges remain in large-scale, cost-effective manufacturing and long-term stability in biological environments. Additionally, understanding their long-term effects on human health is an area that requires further research. This paper highlights the benefits, challenges, and limitations of nanostructured metals, while suggesting future research directions to improve manufacturing, performance, and integration in medical devices and implants.



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sciforum-114883: Mechanical and tribological evaluation of a biomedical high-entropy alloy reinforced with TiC and TiB

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High-entropy alloys (HEAs) are emerging materials that have recently been considered for biomedical applications. However, further adjustments in their properties are still needed to potentialize this application. Thus, research on novel processing routes is interesting for producing such advanced biomedical HEAs. In this study, we synthesized a novel metal-matrix composite (MMC) using an HEA as the matrix, which was reinforced with TiB and TiC particles. The sample was produced by argon arc melting a TiNbZrTaMo ingot with B₄C powder to induce in situ reactions. The resulting sample underwent extensive evaluations, including physical, chemical, structural, microstructural, mechanical, tribological, and biological assessments, and was compared to the unreinforced HEA sample. X-ray diffraction confirmed the in situ reactions, revealing a dual-phase (BCC + HCP) matrix with TiC and TiB peaks. Scanning and transmission electron microscopy showed that the BCC phase was enriched with refractory metals (Ta, Mo, and Nb), while the HCP and carbide precipitate phases were enriched with Ti and Zr. The results demonstrated strong interfacial bonding between the TiC precipitate and the matrix. Mechanical property analysis indicated that the precipitates retained a combination of high microhardness and a relatively low elastic modulus. Despite this, the precipitates enhanced wear resistance without offering any benefits in terms of corrosion resistance. Cytotoxicity tests showed that the precipitates positively influenced cell viability and adhesion. These findings highlight the potential for developing novel biomedical materials by combining HEA and MMC concepts. (Financial support: CNPq and FAPESP grant #2024/03148-3)



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sciforum-107973: Metal and chelator complexes—A newly discovered technology to purify immunoglobulins without Chromatography, polymers, membranes, or specific ligands.

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We introduce a new concept and a potentially general platform for the purification of immunoglobulins that does not rely on any resins, chromatographic media, membranes, or specific ligands; rather, it makes use of aromatic [metal–chelator] complexes. A hydrophobic chelator is combined with three different metal ions to establish our purification system. We experimented on the purification of IgG, IgM, and IgA, along with an artificial impurity background. Our impurity background contained 2600 proteins, along with 600 membrane proteins. Our system captured the target immunoglobulins quantitatively via [cation– π] and [π – π] interactions and allowed for their recovery at high yields (80% to 88%, by densitometry) and purity (90% to 96%, by SDS-PAGE), while preserving their secondary structure (by circular dichroism, CD, and native PAGE gel electrophoresis) and monomeric state (by dynamic light scattering, DLS). The entire process was performed at pH 6–7, thereby avoiding complications that derive from exposure to harsh acidic conditions (e.g., aggregation, partial denaturation). The potential to upscale the technology was evaluated at the laboratory scale. The leaching of the metal–chelator complex to the eluted antibodies was assessed and found to be less than 1%. The recycling of the chelator after the purification process generated a satisfactory yield of 95–97%. The cost-effectiveness and simple integration into the future, industrial-scale downstream processing of therapeutic-grade biopharmaceuticals is discussed.



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sciforum-114947: Study of corrosion behavior of biocompatible porous monolithic material based on titanium nickelide

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Introduction: Corrosion resistance is one of the most important requirements for medical devices, as it determines the service life of the material. The aim of this work is to study the corrosion resistance of new biocompatible porous monolithic materials based on titanium nickelide (TiNi), with a different ratio of the reaction additive in the powder system (TiNi:(Ti-Ni)).

Materials and methods: Porous monolithic samples consisting of a monolithic TiNi plate with a porous powder surface were used as the studied material. The surface was powder mixture A-B, where mixture A was (5%Ti+0.5%Ni+TiNi), with exothermic additive B (Ti+Ni) in various ratios: TiNi (1-1), TiNi (1-0.75), TiNi (1-0.5). Sintering was carried out at a temperature of 1100 °C and was held for 15 minutes in an electric vacuum furnace. To homogenize the surface, the studied samples were subjected to electron beam treatment. The determination of corrosion resistance was carried out using voltammetry, with a linear potential sweep in a physiological solution.

Results: According to the data obtained from the electrochemical studies, it was established that the rate of corrosion is influenced by the amount of an exothermic additive. The lowest corrosion rate was observed in the TiNi with the highest content: the value of the corrosion rate of the TiNi sample (1-1) was about 2.5 times less than in TiNi (1-0.5). Microscopic analysis showed the presence of local fractures on the surface of the material after electrochemical tests, including cracks and pitting. The porous areas of the material were mainly corroded; therefore, the corrosion rate increases with a decrease in the amount of the exothermic additive.

Conclusions: As a result of the work performed, it is shown that an increase in the proportion of exothermic additives leads to an increase in the corrosion resistance parameters of porous monolithic materials based on TiNi.



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sciforum-114776: Surface Roughness Optimization of CP Titanium for Improved Osseointegration in Dental Implants

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Introduction:

Surface topography plays a critical role in optimizing titanium implants for enhanced osseointegration—a phenomenon first described by Prof. Brånemark in 1952. His pioneering discovery led to dental implants with a surface roughness (Ra) of approximately 0.15 µm achieved through electropolishing. Advances in bone fixation have since introduced various surface treatments to improve implant roughness favouring cell adhesion. This study investigates the roughness of commercially pure (CP) titanium treated with electrochemical oxidation coatings to assess their suitability for dental applications.

Methods:

CP titanium specimens (n=6) underwent surface coating via a proprietary electrochemical oxidation (ECO) of Biocera Medical (WO 2020/049299) in phosphate–zirconate electrolyte with four different concentrations of zinc (Zn) additive: Type 1 (Zr-P), Type 2 (Zr-P-Zn (L)), Type 3 (Zr-P-Zn (M)), and Type 4 (Zr-P-Zn (H)). Surface roughness of applied zirconia–Titania ceramic enriched with P and Zn was measured using a Keyence digital microscope (4 readings per sample) and three-dimensional parameters (Sa, Sq, Sz) following ISO 25178.

Results:

Coated titanium surfaces demonstrated increased roughness compared to uncoated titanium (Sa = 0.45 ± 0.07 µm). Coating Type 1 had a minimal impact on roughness (Sa = 0.49 ± 0.09 µm), while Types 2, 3, and 4 increased the mean Sa values to 0.63 ± 0.07 µm, 0.66 ± 0.05 µm, and 0.72 ± 0.10 µm, respectively. The roughness is not homogeneous, following lines for uncoated Ti while it is more spotted for coated samples, as observed on 3D Sa maps.

Conclusions:

Electrochemical oxidation coatings enriched with Zn increased the roughness of CP Ti surfaces. The higher roughness of Types 2–4 may enhance osseointegration by promoting cell attachment and therefore would improve titanium's surface properties for dental implants. Further research will expand the analysis of coating properties with SEM/EDS imaging, nano-indentation, and biological performance.



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