CMDWC 2022

The 2nd Corrosion and Materials Degradation Web Conference

05–07 JULY 2022 | ONLINE

Program and Abstract Book

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Session Chairs

Prof. Dr. Digby Macdonald	Prof. Dr. Homero Castaneda	Dr. Scott Wade
Prof. Dr. David M. Bastidas	Dr. Parama Banerjee	Prof. Dr. Raman Singh
Prof. Dr. Daniel John Blackwood	Prof. Dr. Andrej Atrens	Dr. Vijayshankar Dandapani
Prof. Dr. Mikhail Zheludkevich	Prof. Dr. Dominique Thierry	Dr. Sviatlana Lamaka

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Conference Secretariat

Ms. Lilith Wu
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Welcome from the Chairs

It is our great pleasure and honor to invite you to the "2nd Corrosion and Materials Degradation Web Conference" (CMDWC 2022), a conference organized by the MDPI open access journal Corrosion and Materials Degradation (CMD).
Following the very successful 1st conference (https://cmdwc2021.sciforum.net/), we are pleased to present CMDWC 2022, which will allow attendees to actively engage in discussions about the latest findings in the field. Scientists or engineers working on corrosion are encouraged to join this event and share their findings on the following general and related themes:

- Session 1: Electrochemical Corrosion Mechanism at the Interface (Localized, Crevice, Advanced Characterization Techniques, EAC, Nanoscale)
- Session 2: Corrosion of Steel in Concrete
- Session 3: Computational Modelling, Design and Prediction of Corrosion
- Session 4: Surface Treatments and Coatings for Corrosion Protection
- Session 5: Corrosion in New Materials (HEA, CCA, TWIP/TRIP, AM, PM)
- Session 6: Corrosion in the Energy Sector (Renewable and Nuclear)
- Session 7: Corrosion in Biomedical Implants
- Session 8: Atmospheric Corrosion
- Session 9: Microbiologically influenced Corrosion
- Session 10: Corrosion of Magnesium Alloys
- Session 11: Corrosion Inhibition

During the three-day conference, numerous internationally renowned speakers will share their current state-of-the-art research, along with selected talks from the abstracts received. A quick tour of the 1st conference (https://cmdwc2021.sciforum.net/) will show that we successfully achieved our mission. Each CMDWC 2022 session will include comprehensive and vibrant Q&A sessions. Submitted abstracts will be reviewed by the conference committee. All accepted abstracts will be available for registered participants in the form of a book of abstracts during the conference period. At the conference, authors will also have the option to produce short video presentations.

We look forward to welcoming you to this exciting event.

Prof. Dr. Raman Singh
Conference Chair

Prof. Dr. Digby Macdonald
Conference Chair

Prof. Dr. David M. Bastidas
Conference Chair

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General Information

corrosion and materials degradation

an Open Access Journal by MDPI

Corrosion and Materials Degradation is an international, peer-reviewed, open access journal on corrosion, environment-assisted degradation, corrosion mitigation, corrosion mechanism and corrosion monitoring, published quarterly online by MDPI. Among other databases, *Corrosion and Materials Degradation* is indexed by CNKI, DOAJ, EBSCO, Gale, J-Gate, OpenAIRE, PATENTSCOPE and ProQuest.

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Rapid Publication: manuscripts are peer-reviewed and a first decision provided to authors approximately 27.7 days after submission; acceptance to publication is undertaken in 4.6 days (median values for papers published in this journal in the second half of 2021).
Recognition of Reviewers: APC discount vouchers, optional signed peer review, and reviewer names published annually in the journal.

Program

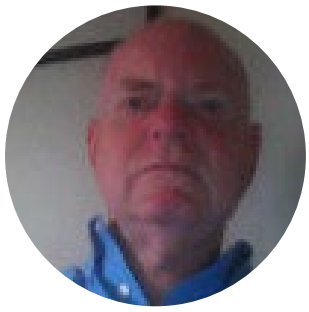
Keynote Speakers

Prof. Dr. Andrej Atrens
The University of Queensland, Australia

Prof. Dr. Herman Terryn
Vrije Universiteit Brussel, Belgium

Prof. Dr. Xosé Ramón Nóvoa
Universidade de Vigo, Spain

Prof. Dr. Derek Lovley
University of Massachusetts, Amherst,, USA



Dr. Anthony Hughes
CSIRO Mineral Resources, Australia

Prof. Dr. Marjorie Olivier
Université de Mons, Belgium

Dr. Ivan Cole
Royal Melbourne Institute of Technology (RMIT), Australia

Prof. Dr. Arjan Mol
Technische Universiteit Delft, The Netherlands

Prof. Dr. Philippe Marcus
Centre National de la Recherche Scientifique, France

Prof. Dr. Mikhail Zheludkevich
Helmholtz-Zentrum Hereon, Germany

Invited Speakers

Prof. Dr. Homero Castaneda
Director of the National Corrosion and Materials Reliability Center, Texas A&M University, USA

Dr. Carmen Andrade
International Center for Numerical Methods in Engineering (CIMNE) - UPC, Spain

Prof. Dr. Florin Bobaru
University of Nebraska-Lincoln, USA

Dr. Pierangela Cristiani
Ricerca sul Sistema Energetico, Italy

Prof. Dr. Kathleen Duncan
University of Oklahoma, USA

Prof. Dr. Regine Willumeit-Römer
Institute of Materials Research, Metallic Biomaterials, Helmholtz-Zentrum Geesthacht, Germany

Dr. Dan Persson
RISE Research institute, Sweden

Prof. Dr. Frank Witte
Geriatric Dentistry and Craniomandibular Disorders, Charité, Germany

Dr. Endzhe Matykina
Complutense University of Madrid, Spain

Dr. Peng-Wei Chu
National Tsing Hua University, Taiwan

Dr. Parama Chakraborty Banerjee
Geriatric Dentistry and Craniomandibular Disorders, Charité, Germany

Prof. Dr. Ime Bassey Obot
King Fahd University of Petroleum and Minerals, Saudi Arabia

Dr. Jeffrey Venezuela
The University of Queensland, Australia

Dr. Christopher D. Taylor
Ohio State University (OSU), USA

Prof. Dr. Jaroslaw Drelich
Materials Science and Engineering, Michigan Tech, USA

Ms. Zahrina Mardina
The University of Queensland, Australia

Prof. Dr. Yufeng Zeng
College of Engineering, Peking University, China

Program at a Glance

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Conference Program

Day 1 - Tuesday, 05 July 2022, 08:35 - 18:20 (CEST)

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09:10 - 09:35	**Prof. Dr. Jaroslaw Drelich** *Corroding Zinc Scaffolds: Using Art of Metallurgy to Combat Vascular Diseases*
09:35 - 10:00	**Prof. Dr. Yufeng Zeng** *The corrosion behavior of pure Zn in simulated body fluids*
10:00 - 10:25	**Prof. Dr. Frank Witte** *Recent development in biodegradable Mg implants*
10:25 - 10:35	**Dr. Jeffrey Venezuela** *Developing Biodegradable Zn-Ca-Cu alloys for Wound Closure Applications*
10:35-10:45	**Ms. Zahrina Mardina** *The prospect of biodegradable metallic mesh for pelvic floor reconstruction: dynamic behaviour point of view*
10:45-10:55	**Dr. Alina Vladescu** *Effect of deposition temperature on properties of hydroxyapatite coatings deposited on biodegradable AZ31B alloy*
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10:55 – 11:00 Break time	
S11. Corrosion Inhibition Chair: Dr. Sviatlana Lamaka	
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11:30 - 12:00	**Prof. Dr. Arjan Mol** *Laying the experimental foundation for machine learning in corrosion inhibitor discovery*
12:00 - 12:30	**Prof. Dr. Anthony Hughes** *Investigating the Microstructure and Corrosion of Additively Manufactured Steels with a View to Protection*
12:30 - 13:00	**Dr. Endzhe Matykina** *Evaluation of the effect of ciprofloxacin loaded into hybrid oxide-polymer coating on corrosion of Mg3Zn0.4Ca alloy*
	Q&A included in each time slot
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S3. Computational Modelling, Design and Prediction of Corrosion Chair: Prof. Dr. Daniel John Blackwood	

13:50 - 14:15	**Prof. Dr. Herman Terryn** *Comparing Modelling and Experiments for Prediction of Atmospheric Corrosion under Controlled Dynamic Thin Film and Droplet electrolytes*
14:15 - 14:35	**Prof. Dr. Florin Bobaru** *Crevice and Galvanic Corrosion: Benefits from Peridynamic Models*
14:35 - 14:55	**Prof. Dr. Ime Bassey Obot** *Materials Degradation Control using Corrosion Inhibitors: From Computational Modeling to Laboratory Development*
14:55 - 15:15	**Prof. Dr. Christopher Taylor** *From Mechanistic Modeling of Corrosion to Generating Descriptors for Materials Design, Selection and Prediction*
15:15 - 15:20	*Q&A session*
15:20 - 15:30	sciforum-061086 - Aravinth Ravikumar - *A microstructural hydrogen permeation model of ultra-high strength martensitic steels with zinc-nickel coating*
15:30 - 15:40	sciforum-060579 - Mohsen Saeedikhani - *Finite Element Method to Better Understand and Interpret Scanning Vibrating Electrode Technique on Scratched Coatings and Inclined Surfaces*
15:40 - 15:50	sciforum-058326 - Andrey Krauklis - *Modelling Hydrolytic Degradation of the Composite Interphase in a Modular Manner*
15:50 - 16:00	sciforum-061026 - Keith Kee - *Using data analytics and machine learning for non-invasive and non-contact evaluation for corrosion inspection in fixed assets (such as tanks and buried pipelines) and rotating equipment (example, pumps and generators)*
16:00 - 16:05	*Q&A session*
	16.05 -16.25 Break time
	S2. Corrosion of Steel in Concrete **Chair: Prof. Dr. David M. Bastidas**
16:25 - 17:00	**Prof. Dr. Xosé Ramón Nóvoa** *The behaviour of reinforced concrete elements under loading. An EIS study*
17:00 - 17:20	**Prof. Dr. Homero Castaneda** *Mechanistic Determination of Chloride Threshold of Cr-based Steel Rebars in Simulated Concrete Pore Solution (SCPS) based on Electrochemical Methods*
17:20 - 17:40	**Prof. Dr. Carmen Andrade** *XANES study of early stages of steel corrosion in alkaline media simulating concrete pore solution*

Day 2 - Wednesday, 06 July 2022, 08:45 - 16:50 (CEST)

S9. Microbiologically influenced Corrosion Chair: Dr. Scott Wade	
08:45 - 09:20	**Prof. Dr. Derek Lovley** *Mechanisms for Microbially Enhanced Metal Corrosion Under Anaerobic Conditions*
09:20 - 09:45	**Dr. Pierangela Cristiani** *Evolution of microbial corrosion research from the previous century to the present*
09:45 - 10:10	**Prof. Dr. Kathleen Duncan** *Microbial Communities Associated with Carbon Steel Corrosion in Model Seawater Compensated Fuel Ballast Tanks*
	Q&A included in each time slot
10:10 - 10:20	sciforum 060942- Laura Munoz - *The role of H2 on the acetogens influenced corrosion*
10:20 - 10:30	sciforum-059750 - Xiao Deng - *Uptake of low-energy electrons from electrodes in Desulfovibrio vulgaris Hildenborough*
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S4. Surface Treatments and Coatings for Corrosion Protection Chair: Prof. Dr. Mikhail Zheludkevich	
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11:35 - 11:45	sciforum-060879 - Borja Pillado - *Functionalized hybrid PEO/Sol-gel Coatings for corrosion protection of Mg alloys*
11:45 - 11:55	sciforum-060645 - Manasa Hegde - *Abrasion and cavitation erosion resistance of multi-layer dip coated sol-gel coatings on AA2024-T3*
11.55-12.05	sciforum-061018 - Peter Rodič - *Corrosion protection of AlSi7Mg0.3 using zirconium conversion treatment and polyacrylate siloxane-silica sol-gel coating*
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12.10-12.20	sciforum-060687 - Elias KAADY - *The effect of ALD oxides thin films on the electrochemical properties of the sputtered Al-Zr coatings*
12:20-12:30	sciforum-060666 - Stanley Ofoegbu - *Effect of Sealing Temperature on the Corrosion Resistance and Mechanical Properties of Sulphuric Acid Anodized 6060 Aluminium Alloy.*
12.30-12.40	sciforum-060880 - Esther López - *Characterization, Surface Modification and Performance of an Additive Manufactured Al alloy*
12.40-12.45	*Q&A Session*
12:45 - 14:00 – Lunch Break	
S8. Atmospheric Corrosion Chair: Prof. Dr. Dominique Thierry	
14:00 - 14:35	**Dr. Ivan Cole** *How to link Molecular Level -Inhibitor Surface Reactions with Continuum -Electrochemical Response: Quantitative structure-activity relationship or Expanded Molecular Models*

	Dr. Dan Persson
14:35 - 15:00	*Infrared-spectroscopy-based techniques for studies of atmospheric corrosion and degradation of coated materials*
15:00 - 15:10	sciforum-059237 - Isabel Fontinha - *Influence of exposure conditions and particulate deposition on anodized aluminum corrosion*
15:10 - 15:20	sciforum-060988 -- Firdausi Zamrudi - *Atmospheric corrosion of dissimilar friction stir welded AA2017 and AA7075 in urban area of Indonesia*
15:20 - 15:30	sciforum-060999 -- Jasmita Nur Azizah - *Study of Atmospheric Corrosion Characteristics of Magnesium Alloy AZ31B in Tropical Rural and Urban Environments*
15:30 - 15:45	*Q&A Session*
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	S5. Corrosion in New Materials (HEA, CCA, TWIP/TRIP, AM, PM) **Chair: Prof. Dr. Homero Castaneda**
	Dr. Wenjun (Rebecca) Cai
16:15 - 16:50	*Corrosion of Lightweight Concentrated Alloys: Roles of the Passivating vs. Non-Passivating Elements*
	Q&A included in each time slot

Day 3 - Thursday, 07 July 2022, 08:45 - 13:00 (CEST)

S6. Corrosion in the Energy Sector Chair: Dr. Parama Banerjee	
8:45-8.55	sciforum-057802 - Kerman Vázquez - *Corrosion Prediction Models in the Reinforcement of Concrete Structures of Offshore Wind Farms*
8.55-9.05	sciforum-060866 - RISHIKESH K V - *Evaluation of long exposure behavior of IN617 under high temperature and high-pressure air and steam environments*
9.05-9.15	sciforum-060890 - Wenye Lin - *Compatibility of different metallic materials and a novel salt hydrate phase change material slurry as secondary refrigerant for building air conditioning*
9.15-9.25	*Q&A Session*
9.25-9.35	sciforum-060968 - Julio José Caparrós Mancera - *Experimental characterization of aluminum exposed to acid mine drainage corrosion*
9.35-9.45	sciforum-060986 - Miftahul Jannah - *Effects of pH and zwavelzure amoniak (ZA) fertilizer on the corrosion resistance of X60 steel in soils*
9.45-10.00	*Q&A Session*
10:00 - 11:00 – Coffee Break	
S10. Corrosion of Magnesium Alloys Chairs: Dr. Vijayshankar Dandapani and Prof. Dr. Raman Singh	
11.00-11.35	**Prof. Dr. Andrej Atrens** *Mg Corrosion–recent progress*
11.35-12.10	**Prof. Dr. Mikhail Zheludkevich** *Complexants as active modulators of Mg surface reactivity*
12.10-12.35	**Dr. Peng-Wei Chu** *Microstructure of the Surface Corrosion Film on Biodegradable Mg Alloys in Simulated Body Fluids*
12:35 - 13:00	**Dr. Parama Banerjee** *Corrosion in magnesium batteries: Current challenges and future perspectives* **Q&A included in each time slot**
Closing Remarks Chairs: Prof. Dr. Raman Singh, Prof. Dr. Digby Macdonald & Prof. Dr. David M. Bastidas	

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Sciforum is an event planning platform that supports open science by offering the opportunity to host and participate in academic conferences. It provides an environment for scholarly exchange, discussion of topics of current interest, building of networks and establishing collaborations.

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Abstracts

Session 1. Electrochemical Corrosion Mechanism at the Interface (Localized, Crevice, Advanced Characterization Techniques, EAC, Nanoscale)

No Abstracts in this session

Abstracts

Session 2. Corrosion of Steel in Concrete

Sciforum-060842: Cationic Species Effect on the Corrosion Inhibition Performance of NO2–/NO3– on Steel Reinforcements

Ahmed Mohamed[1], Donald P Visco Jr[1], David M Bastidas[1]

[1] The University of Akron

Two different cationic species, Na^+ and Ca^{2+}, were tested for NO_2^-/NO_3^- corrosion inhibitors on steel reinforcements in 0.6 M Cl^- contaminated simulated concrete pore solution at 25, 35, 45, and 55 ºC. Electrochemical monitoring was utilized to understand the effect of cationic species on the inhibition performance of the corrosion inhibitors. Experimental results showed that NO_2^-/NO_3^- corrosion inhibitors had strong anti-corrosion performance achieving IE of 85, 78, 71, and 59% for $NaNO_2$, $Ca(NO_2)_2$, $NaNO_3$, and $Ca(NO_3)_2$, respectively, at 25 ºC. It was found by potentiodynamic polarization and electrochemical impedance spectroscopy that at every temperature the best corrosion inhibitor was $NaNO_2$ followed by $Ca(NO_2)_2$, $NaNO_3$, and $Ca(NO_3)_2$. The thermodynamics of activation of the corrosion process revealed that the activation energies, enthalpies, and entropies of the corrosion inhibitors were greater than the blank due to the adsorption mechanism, endothermic dissolution of the rebar, and increased energy dispersal from the displaced water molecules around the rebar from the adsorbed inhibitor molecules. Finally, a trend was observed where Na^+ salts of NO_2^-/NO_3^- corrosion inhibitors were performing better than Ca^{2+} salts. Hence, the activity coefficients of ions in solution were calculated utilizing the Pitzer model and it was found that Ca^{2+} salts decreased the activity of NO_2^-/NO_3^- ions compared to Na^+ salts, thus explaining the difference in corrosion inhibition performance.

Sciforum-063592: Mechanistic Determination of Chloride Threshold of Cr-based Steel Rebars in Simulated Concrete Pore Solution (SCPS) based on Electrochemical Methods

Homero Castaneda- Lopez[1]

[1] Materials Science and Engineering, Director of the National Corrosion and Materials Reliability Center, Texas A&M University, USA

Steel rebars have been widely applied in reinforced concrete (RC) structures due to their improvements in mechanical properties as a composite material. However, exposure to chemical aggressive ions such as chloride ions and oxygen originates a corrosive cell that causes the material loss of the rebar and therefore the loss of capacity required for structural elements. The literature has reported a significantly wide range of chloride threshold (CT) based on different laboratory methodologies and theoretical approaches. This work aims to provide a quantitative CT for steel rebars with different Cr content by using the expression of free chloride in wt% and [Cl-]/[OH-] by conducting electrochemical testing (EIS and cyclic polarization) and corroborating with high-resolution image and surface characterizations (SEM and XPS). The added chloride ions were controlled by using several chloride concentrations to detect and characterize the passive to an active mechanism based on quantitative results.

Sciforum-058570: Environmentally Assisted Cracking Mechanisms Of Duplex Stainless Steel Reinforcements In Chloride Contaminated Environment

Ulises Martin Diaz[1], D.M. Bastidas[1]

[1] The University of Akron

The need for more corrosion-protective and long-lasting materials for the construction and building industry in marine environments has led to the use of new stainless steels (SSs). Recently, constructions of great magnitude, such as the Hong Kong–Zhuhai–Macau Bridge (constructed in 2018) with service lifetime predictions of 120 years or the Second Gateway Bridge in Australia (constructed in 2010) with 300 years, used SS reinforcements in the splash zone and key locations. Initially, AISI 304 and AISI 316 austenitic SS rebars were used because they provided considerable improvements in corrosion protection compared to carbon steel. More recently, duplex SS (DSS) reinforcements were developed, such as DSS 2205, which has lower nickel content compared to austenitic SS but improves its yield strength and pitting corrosion performance.

In this work, the stress corrosion cracking (SCC) mechanism of lean DSS 2001 was studied by means of the slow strain rate technique. The SS rebars were tested as a function of the chloride content in a simulated concrete pore solution (pH 12.6). The study of the formation and breakdown of the passive film is carried out through non-destructive electrochemical tests (electrochemical impedance spectroscopy (EIS)) as well as through current transient (with an applied potential of +200 mV_{SCE}). The semiconductive properties of the passive film were analyzed by Mott–Schottky and correlated with the fitted elements of the EIS. The microstructure and the ratio between austenite and ferrite were studied by X-ray diffraction (XRD) and electron backscattered diffraction (EBSD), paying careful attention to the pit nucleation and further crack propagation. Inspection using a scanning electron microscope (SEM) on the fracture area and on the cross-section was carried out to further unravel the crack path.

Sciforum-060878: The behavior of reinforced concrete elements under loading: An EIS study

Belén Díaz[1], X. Ramón Nóvoa[1], Carmen Pérez[1]

[1] Universidade de Vigo

Concrete is a material of porous nature that, when humidified, becomes an ionic conductor whose apparent conductivity depends on the ionic load (typically based on OH-, Ca2+, Na+, K+) and the amount of available free water. Under conditions of partial pore-saturation, the amount of free water can be modulated by an external load, which leads to observable changes in electrical properties, such as conductivity and capacitance. Moreover, the presence of metallic reinforcements, either as bars or fibers, represents an additional parallel conduction path but of electronic nature in this case. The free water develops a double layer capacitance structure at the metallic interfaces, with associated charge transfer resistance, that represents an additional contribution to the capacitive behavior that again can be modulated with an external load. The dependence that the electrical and/or ionic conducting properties of concrete and reinforced concrete elements have on the available free water makes them suitable for transductors in various types of sensing and self-sensing applications that will be discussed in the presentation.

Sciforum-060558: XANES study of early stages of steel corrosion in alkaline media simulating concrete pore solution

Carmen Andrade[1], German R. Castro[2], Sandra Cabeza[3]

[1] International Center for Numerical Methods in Engineering (CIMNE), Spain
[2] European Synchrotron Radiation Facility (ESRF)- BM25-SpLine, France; Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Spain
[3] Institute Laue Langevin, 71 Avenue des Martyrs 38042 Grenoble, France

The pore solution of the concrete is alkaline which induces immediate passivation of the steel of the reinforcement. Corrosion of the steel bars may start if the pH value decreases until neutrality as happens after carbonation of the concrete cover or when chlorides reach the rebar surface in enough amount to induce local corrosion. In both cases it is believed that the corrosion does not initiate if oxygen is not present in the pore solution. However, the corrosion potential values of the steel embedded in concrete indicate stable passivity because they usually are very positive. In the present study XR absorption tests were made of the iron oxides during their initial formation in alkaline solutions without and with chlorides added and with oxygen and using N_2 flow. X-ray scattering data (XANES) were collected at the CRG BM25 SpLine beamline at the European Synchrotron Radiation Facility (ESRF), France with a focused X-ray beam in the energy range between 6.9 and 8.0 keV. The results indicated that only Fe (+3) is detected in the alkaline solutions while both oxidation states (+2 and +3) are detected when chlorides are present in enough amount to produce active corrosion with no distinction when the solution is oxygenated or de-aerated. This indicates that first corrosion is produced with very scarce concentration of oxygen and that the iron species are similar in nature.

Abstracts

Session 3. Computational Modelling, Design and Prediction of Corrosion

Sciforum-061026: Using data analytics and machine learning for non-invasive and non-contact evaluation for corrosion inspection in fixed assets (such as tanks and buried pipelines) and rotating equipment (example, pumps and generators)

Keith Kee[1]

1 President of Corrosion Association Singapore; Formerly Chairman and Trustee of NACE International (Founding Singapore Section)

Fixed assets structures in the energy industry such as large storage tanks and buried underground pipelines will usually require operational down time or shutdown in order for integrity testing to be carried out. For example, checking for corrosion and/or leaks at the bottom annular plate of storage tanks. We are able to perform the inspection use acoustic emission from sensors installed on the external of the tank coupled together with intelligent software for eliminating false positive detection. This is done without requiring empty its content and no tank entry is required.
Rotating equipment such as co-generators and pumps require regular inspection and maintenance to prevent occurrence of unexpected failures resulting in downtime time. Using sound density, we are able to process large datasets of sounds of equipment to detect anomalies in equipment condition. Hence we can use machine learning and artificial intelligence to help predict failure before it happens

Sciforum-060563: From Mechanistic Modeling of Corrosion to Generating Descriptors for Materials Design, Selection and Prediction

Christopher Taylor[1]

[1] Fontana Corrosion Center

Corrosion is a multiscale, multiphysics process. Corrosion reactions transcend time and length scales, as well as classes of materials, and developing predictive models requires in-depth knowledge of metallurgy, surface physics, electrochemistry, mass transport, thermodynamics of speciation, and non-equilibrium thermodynamics. Corrosion mechanisms are also highly sensitive to changes in metallurgy, materials composition, microstructure and perturbations to the environment (pH, chemistry, temperature), and the most significant rate-limiting steps can rapidly change as a function of those variables, making it hard to develop predictive models from first-principles. Mechanistic models can be constructed that follow certain reaction pathways sequentially or in parallel, but their quantitative accuracy is frequently challenged by the limits imposed by requiring the idealization of the system to numerically solvable forms. Recent approaches have sought to circumvent this by identifying key descriptors that characterize aspects of a corrosion mechanism and can be correlated using machine learning or other techniques to quantitative, measurable indicators of corrosion performance. Three examples will be presented in this talk: (1) the correlation of model adsorption isotherm-derived descriptors with the repassivation potential, (2) the correlation of electronic work functions with the open circuit potential, and (3) the correlation of oxygen binding energies to the high-temperature oxidation rate constant.

Sciforum-058326: Modelling Hydrolytic Degradation of the Composite Interphase in a Modular Manner

Andrey Krauklis[1]

[1] Institute for Mechanics of Materials, University of Latvia

Fibre-reinforced composites are used in marine, offshore oil and gas structural applications due to their lightweight and excellent mechanical properties. Exposure of composites to water leads to hydrolytic degradation and environmental ageing, weakening the composite over time. Thus, the superior properties are significantly compromised due to long spans, typically 25–40 years, in contact with the environment. Some common fibres and sizing-rich interphases are prone to hydrolysis. Thus, modelling becomes vital for predicting long-term environmental durability.
Various approaches have been proposed to predict the long-term properties based on short-term measurements (to reduce time and costs). However, the reasons for complexity are the three microconstituents: matrix, fibres, and interphase. Inside a composite, the ageing pathways of individual microconstituents are hard to distinguish. Thus, leading to the necessity of introducing modular or multiscale modelling methods. One such pathway is the Modular Paradigm, which breaks down a complex ageing phenomenon into smaller modules [1-30]. Herein, the Modular Paradigm is applied to study the hydrolytic degradation of the composite interphase. Quantitative modelling is provided and compared with the experimental evidence.
The Modular Paradigm, along with the modelling toolbox, is seen as a valuable tool for predicting the lifetime and accelerated testing. It provides a deeper understanding of the ageing effects on the time-dependent properties of composites and composite interphases.

Keywords: modular paradigm; composite materials; environmental ageing; multiscale modelling; accelerated ageing; lifetime prediction.

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Sciforum-061086: A microstructural hydrogen permeation model of ultra-high strength martensitic steels with zinc-nickel coating

Aravinth Ravikumar[1], Christian Feiler[1], Daniel Höche[1], Mikhail Zheludkevich[1], Manoj Prabhakar[2], Michael Rohwerder[2], Jaime Ochoa Saenz de la Fuente[3], Jorge Rodriguez Jimenez[3], Elena Guinea[3], Maria Lekka[3], Garikoitz Artola[4], Enara Mardaras[4]

[1] Helmholtz Zentrum Hereon, Germany
[2] Max-Planck-Institut
[3] Fundación Cidetec
[4] Azterlan

Electrochemically plated ultra-high strength steels (UHSS) are martensitic steels of high strength with yield limits beyond 1400 MPa. Zn-Ni coatings offer excellent corrosion resistance, as they allow the formation of complex corrosion products that stop the diffusion of corrosive species. The hydrogen in the steel lowers its load bearing and energy absorption ability and this negative effect on the steel's properties is termed as hydrogen embrittlement (HE). HE causes delayed cracking, which might lead to catastrophic material failures.
The prevalent disadvantage of using ultra-high strength martensitic steels is their susceptibility to HE. Herein, a finite element model is developed to capture the transport of hydrogen in plated UHSS during hydrogen embrittlement relief treatment (degassing). Naturally, the morphology of the plating plays an important role in the degassing efficiency and the grain structures, grain boundaries, trapping sites, and residual stresses dictate the diffusion of hydrogen in the steel. Thus, microstructural images are analyzed to understand the microstructure, distribution of the phases and grain structure of the UHSS and the plating and are subsequently utilized to create the geometry of the model. The underlying equations account for the surface reactions leading to the release, reflection back into the steel lattice and inflow due to the difference in partial pressure of hydrogen across the surface. The computational model is calibrated using experimental data for 300M steel with different plating morphologies, and, finally, a workflow is established to determine the concentration of hydrogen in a part after hydrogen embrittlement relief treatment.

Sciforum-062523: Comparing Modelling and Experiments for Prediction of Atmospheric Corrosion under Controlled Dynamic Thin Film and Droplet electrolytes

N. Van den Steen[1], K. Zhang[2], A. Kosari[2], B.G. Koushik[1], Y. Van Ingelgem[1], Y. Gonzalez-Garcia[2], J.M.C. Mol[2], H. Terryn[2]

[1] Department of Materials and Chemistry, Research Group Electrochemical and Surface Engineering (SURF), Vrije Universiteit Brussel, Pleinlaan 2, 1050 Brussels, Belgium
[2] Department of Materials Science and Engineering, Delft University of Technology, Mekelweg 2, 2628 CD Delft, The Netherlands

Corrosion prediction by multiscale modelling aims to achieve the required paradigm shift in the lifetime prediction of metals. Modelling of atmospheric corrosion, for example, based on Finite Element Modelling (FEM) requires an exact description of the boundary region between metal and electrolyte. This requires a radically different research approach for the electrolyte in contact with the metal surface. The critical issue is that most corrosion experiments in fundamental research are performed “in solution” under the assumption that the electrolyte layer is thick enough to approximate it as “infinite”, ignoring significant local effects introduced by dynamic electrolyte dimensions caused by droplets and puddles. In other words, a major part of the research in academia is not relevant to mimic the actual conditions encountered on the metal surface. To create accurate numerical models, we first and foremost needed to abandon this "infinite" and “stationary” approximation and consider dynamic and finite electrolyte dimensions. During atmospheric corrosion of metals, the evolution of the thin-film electrolyte thickness is the primary factor determining the corrosion rate. A full understanding the evolution of the electrolyte thickness and properties as a function of the key environmental parameters is yet to be achieved. A novel methodology has been developed to conduct experiments under a regulated environment to measure the film thickness evolution or individual droplets on an undisturbed metal surface [1]. Experimental results are compared with FEM models predicting both the electrolyte formation, as well as the related corrosion. The heat transfer coefficient is noted as a critical parameter influencing both the film characteristics and the resulting corrosion rate. This model was tested in case of cut-edge corrosion of galvanized steel. Combining the in-house MiTReM (Multi ion Transfer Reaction electrochemical model) with the electrolyte film thickness model, we could see that the corrosion rates become very critical in the range of 20 μm [2]. The next step was to go into the dimension of droplets. A thorough literature review [3] was made and published around modelling of droplet formation and corrosion, forming a base for further progress and improvements. The literature study also highlighted that the topic of droplet formation is relatively new within the corrosion research community.

A new approach [4] was proposed to numerically predict and study atmospheric corrosion under droplet size distributions. The proposed methodology allows for a corrosion prediction based on observed droplet size distributions and droplet contact angles. A mechanistic finite element model, including oxygen transport and Butler–Volmer kinetics, is solved to obtain the current density for the droplet geometry. This is done for a range of both droplet radii and contact angles. The computed corrosion current densities are then adapted onto imposed droplet distributions for a calculation of overall corrosion current. This allows for a calculated material loss estimation for different distributions and electrolyte configurations and shows the extent of the impact of the droplet distribution on atmospheric corrosion. This model is validated by comparing with experiments introducing droplet-

induced corrosion in a lab scale reactor that allows monitoring in parallel droplet geometry and corrosion as function of induced thermal cycles in a controlled atmosphere.

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Sciforum-062499: Crevice and Galvanic Corrosion: Benefits from Peridynamic Models

Florin Bobaru[1]

[1] Professor and Hergenrader Distinguished Scholar, Mechanical and Materials Engineering, University of Nebraska-Lincoln, USA

Crevice and galvanic corrosion are particularly dangerous types of localized corrosion that can lead to fracture and catastrophic failure. Computational modeling of crevice corrosion, for example, is complicated by the extreme aspect ratio of crevices, which are long and narrow spaces. Crevice corrosion attack mostly happens at the mouth of the crevice, where deep trenches can be observed. Outside of that particular region, corrosion is relatively minor, but it cannot be ignored, since it influences what happens near the crevice mouth. A recent peridynamic model for crevice corrosion is able to predict its evolution in great detail [1]. Deep trenches are obtained near the crevice mouth in an autonomous way, by only using far-field boundary conditions. We are able to explain the reason for this seemingly peculiar behavior of corrosion. In galvanic corrosion, high corrosion rates are induced near the metal–metal interface and accurate representation of the electric potential is critical in obtaining predictive results. We have recently showed that classical models require an artificial step be created in the geometry of the bi-material in order to obtain results similar to those seen in experiments [2]. Without this artifice, results from classical models of galvanic corrosion produce misleading smooth damage profiles, hiding potentially dangerous sharp corrosion attack that could easily trigger crack growth and catastrophic failure. The peridynamic (PD) model for galvanic corrosion is able to predict the correct damage profiles caused by galvanic corrosion without the need to change the sample's geometry. This is because the PD model uses a mathematical formulation that eliminates various singularities present in classical models defined on particular geometrical configurations. If time permits I will also present some recent results with a new, fast convolution-based method for PD models of corrosion, able to consider hundreds/thousands of growing pits and samples sizes in the mm/cm scale.

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Sciforum-060579: Finite Element Method to Better Understand and Interpret Scanning Vibrating Electrode Technique on Scratched Coatings and Inclined Surfaces

Mohsen Saeedikhani[1], Daniel John Blackwood[2]

[1] Research Fellow, National University of Singapore
[2] A/Prof, National University of Singapore

The application of the Scanning Vibrating Electrode Technique (SVET) for corrosion studies was started by the pioneering work of Isaacs. Thereafter, a boom began on the use of SVET to investigate the localized galvanic cells that are often responsible for localized corrosion phenomena. Here, some of the problems associated with the interpretation of data obtained from Scanning Vibrating Electrode (SVET) will be discussed.
The SVET is a valuable method for investigating localized corrosion, which has the potential to provide further insights if used in conjunction with simulation. This paper demonstrates, by combining experimental data with finite element simulations, that variation in the height of the probe to the electrode surface will cause an imbalance in the measured anodic and cathodic currents, with IR drop being a main determining factor. In addition, the simulations obtain the actual current density at/across the electrode's surface, whereas the electrolyte current density is obtained by SVET. The galvanic corrosion at scratched and cut-edge zinc-based coated steel in a saline solution are used as examples.
Ref.: M. Saeedikhani et al., *Journal of The Electrochemical Society*, 2021 168 081505.

Sciforum-062498: Materials Degradation Control using Corrosion Inhibitors: From Computational Modeling to Laboratory Development

Ime Bassey Obot[1]

[1] Interdisciplinary Research Center for Advanced Materials, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia

The total estimated cost of downhole oil and gas production corrosion problems in Saudi Aramco, for instance, was USD 2.29 billion in 2009. One of the approaches to mitigating corrosion in the oil and gas industry is the use of corrosion inhibitors. The design, development, and performance evaluation of corrosion inhibitors for the oil and gas industry are primarily conducted by trial-and-error approaches using experimental methods, such as weight loss, linear polarization (LPR), potentiodynamic polarization (PDP), and electrochemical impedance spectroscopy (EIS) measurements using the so-called bubble test and very expensive high-temperature and high-pressure autoclave systems. These experimental methods are tedious, costly, time-consuming, and often do not lead to the fast discovery of potent corrosion inhibitor active molecules. With the advancement in Computational Chemistry and Machine Learning, the use of computer and data-led approaches in the design and development of novel corrosion inhibitors faster is becoming increasingly vital. In this presentation, I will cover the following: material degradation due to corrosion, corrosion inhibitor's field of application, corrosion inhibitor development—past, current, and future—and, finally, the future challenges for corrosion inhibitor development will be highlighted.

Sciforum-060039: Study of Surface-Dependent Corrosion of Fe by Combining the Density Functional Theory and Experiments

Hongmei JIn[1], Daniel John Blackwood[2], Ying Wang[2], Man-Fai Ng[1], Teck Leong Tan[1]

[1] Institute of High Performance Computing, Agency for Science, Technology and Research, 1 Fusionopolis Way, #16-16 Connexis, Singapore 138632, Singapore
[2] 2Department of Materials Science and Engineering, National University of Singapore, 9 Engineering Drive 1, Singapore 117575, Singapore

Combining density functional theory calculation with the Butler–Volmer equation, the corrosion potential and corrosion current for Fe were investigated in this study. The relationship between the electrode potential and the current density in the Butler–Volmer equation was described by using surface energy density, surface work function, atom escape energy and hydrogen adsorption free energies. Polarisation curves were obtained based on the derived relationship. For the anodic branch of the polarisation curve, the equilibrium potential was correlated to surface work function, and atom escape energy and surface energy density were correlated to atom dissolution activation energy in the equation. For the cathodic branch of the polarisation curve, hydrogen adsorption free energy was correlated to the exchange current density. All the parameters in the formulae were derived from density functional theory calculations. The theoretical scheme was applied to investigate the surface-dependent corrosion of BCC Fe and Fe-alloys, and a general agreement was obtained between calculation results and experiment, indicating the reliability of the model. The same approach was further extended to FCC Fe, and the results were compared.

Abstracts

Session 4: Surface Treatments and Coatings for Corrosion Protection

Sciforum-060645: Abrasion and cavitation erosion resistance of multi-layer dip coated sol-gel coatings on AA2024-T3

Manasa Hegde[1], Yvonne Kavanagh[2], Brendan Duffy[3], Edmond F Tobin[1]

[1] Department of Aerospace, Mechanical and Electronic Engineering, Institute of Technology Carlow
[2] Institute of Technology Carlow
[3] CREST, Technological University Dublin

AA2024-T3 are widely used in various applications because of their exceptional physical properties. However, they are susceptible to corrosion and cavitation erosion in aggressive environments due to high concentration of copper. Sol-gel coatings in the field of corrosion prevention are emerging. Improved thickness of coatings significantly improves the barrier effect of the coatings, thereby improving their operational-life in industrial applications. To date, a limited amount of work has been carried out in determining the effect of hybrid sol-gel coatings on abrasion and cavitation erosion of AA2024-T3. The present study investigates the effect of thickness of the coatings on structure, morphology, anticorrosion, abrasion, and cavitation erosion properties of the prepared hybrid sol-gel coatings deposited on AA2024-T3 surfaces. The hybrid sol-gels have been synthesised from 3-trimethoxysilylpropylmethacrylate (MAPTMS), and a zirconium complex prepared from the chelation of zirconium n-propoxide (ZPO), and methacrylic acid (MAAH). AA-2024 T3 were coated using single-dip, double-dip and triple-dip. Attenuated total reflectance–Fourier transform infrared (ATR–FTIR) spectroscopy was performed to indicate the formation of the Si–O–Si structural backbone of the hybrid coatings. Abrasion and cavitation erosion tests were performed according to the relevant standards. Structural damage caused by corrosion, abrasion, and cavitation erosion was studied by Optical Microscope and Scanning Electron Microscope (SEM). Furthermore, mechanical characterization of the coatings was performed by pencil scratch hardness and cross-cut adhesion test. Water contact angle was used to determine the hydrophobicity of the coatings. Corrosion protection performance of the coatings was tested using Open Circuit Potential (OCP) and Potentiodynamic polarization (PDS). Results indicated that the multilayer coated samples improved the corrosion, cavitation erosion and abrasion resistance of AA2024-T3. Hence, the prepared silica-based coatings can be proposed as a potential choice for marine renewable energy applications.

Sciforum-059591: Bioresorbable self-healing coatings for corrosion protection of magnesium implants

Valeriia S. Filonina[1], Andrey S. Gnedenkov[1], Sergey L. Sinebryukhov[1], Sergey V. Gnedenkov[1]

[1] Institute of Chemistry FEB RAS

Improving the electrochemical properties of bioabsorbable magnesium implants will make it possible to control the process of material degradation to match the osteogenesis, as well as to avoid intense alkalization of the surrounding area [1,2]. Protective composite inhibitor-containing coatings obtained on an MA8 magnesium alloy during the presented study allows reducing corrosion destruction in chloride-containing electrolytes (including human body fluids). The basis for forming the composite layers was a hydroxyapatite-containing plasma electrolytic oxidation (PEO) coating. The self-healing ability was realized through the impregnation of the formed layers with stearic acid (SA). To improve the electrochemical properties of an MA8 alloy, the following methods were established:
CC-P—composite coating obtained by two-fold treating the PEO-layer with a 6 wt.% solution of polycaprolactone (PCL) in dichloromethane;
CC-2SP—composite coating formed by impregnating the PEO-layer with stearic acid (0.1 M) from a mixed solvent containing water and ethanol (1:1) with the following two-fold treatment with PCL from a dichloromethane-based solution (6 wt.%);
CC-1SP—composite coating obtained by two-fold dipping the PEO-layer into a solution of SA (0.1 M) and PCL (6%) based on dichloromethane.
Using traditional electrochemical methods (EIS, PDP), it was revealed that samples with CC-2 SP have the best protective properties. The values of corrosion current density for these samples (I_C = 17 nA/cm^2) were by one and two orders of magnitude lower than the ones for CC-1SP and CC-P, respectively. The maximum value of the impedance modulus ($|Z|_{f=0.1\ Hz}$ = 105 kΩ·cm^2) was detected for CC-2SP and was two- and six-folds higher than $|Z|_{f=0.1\ Hz}$ for, respectively, CC-1SP and CC-P. The small discrepancy in the data established by EIS and PDP is a result of the different polarization modes of these techniques, which results in a change in the surface morphology of the samples.
This work was supported by a Grant from the Russian Science Foundation (project no. 20-13-00130).
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Sciforum-060977: Improving the corrosion resistance of orthodontic alloys with a-C:H-based coatings

António Fróis[1, 2], Ana Cristina Santos[3, 4], Cristina Santos Louro[5]

[1] CEMMPRE, Department of Mechanical Engineering, University of Coimbra
[2] Coimbra Institute for Clinical and Biomedical Research/Center for Innovative Biomedicine and Biotechnology (iCBR/CIBB), Biophysics Institute, Faculty of Medicine, University of Coimbra, 3000-548 Coimbra, Portugal;
[3] Coimbra Institute for Clinical and Biomedical Research/Center for Innovative Biomedicine and Biotechnology (iCBR/CIBB), Biophysics Institute, Faculty of Medicine, University of Coimbra, 3000-548 Coimbra, Portugal
[4] Area of Environment Genetics and Oncobiology (CIMAGO), 3000-548 Coimbra, Portugal
[5] CEMMPRE, Department of Mechanical Engineering, University of Coimbra, 3030-788 Coimbra, Portugal

Oral cavity is an ultimate corrosion-promoting environment for bioalloys. Therefore, solutions are needed. Looking for a safe solution to improve human health, a surface engineering approach was chosen for this study: the outstanding diamond-like carbon coatings. In addition to suitable hardness and tribological properties, C-based materials present other desirable characteristics for orthodontics, including bioinertness and electrical insulating character by hydrogen addition. In this work, hydrogenated amorphous carbon (a-C:H) coatings were deposited on stainless steel (SS) substrates by a reactive magnetron sputtering with two CH_4 flows. A 30-day immersion test in artificial saliva was conducted to mimic acidic and neutral intraoral pH values, and the released Ni, Cr, and Fe were quantified by ICP-OES. Characterization by SEM/EDS, Raman, nanohardness and static contact angles revealed no important structural/mechanical changes, regardless the H content (~28 and 40 at.%), without corrosion signs, delamination, or detachment. Moreover, in vitro assays with mono- an co-cultures of macrophages and fibroblasts revealed higher biocompatibility for the lowest H content. However, the Cr-based interlayer used may reduce the corrosion resistance of the coatings. Results will be compared to those obtained by in vivo saliva sampling of patients under fixed orthodontic treatment, considering a Ni and Cr daily intake content up to 300 μg/day.

Sciforum-060974: Novel Hybrid polyphosphate material incorporated in alkyd coating for enhanced corrosion resistance of carbon steel in NaCl

Chaymae Hejjaj[1], Ahmed Ait Aghzzaf[2], Nico Scharnagl[3], Mikhail L. Zheludkevich[3, 4], Rachid Hakkou[5, 6], Christian B. Fischer[7, 8], Jones Alami[7]

[1] Materials Science Energy and Nano-engineering Department, University Mohammed VI Polytechnic (UM6P), Lot 660-Hay Moulay Rachid, 43150, Ben Guerir, Morocco 2 IMED-Lab, Faculty of Science and Technology, Cadi Ayyad University (UCA), BP549, Marrakesh, Mor
[2] Laboratory of Applied Sciences and Didactic (LaSAD), Ecole Normale Supérieure, Abdelmalek Essaadi University, Tetouan, Morocco
[3] Institute of Surface Science, Helmholtz-Zentrum hereon GmbH, Max-Planck-Straße 1, 21502 Geesthacht, Germany
[4] Faculty of Engineering, Kiel University, Kaiserstraße 2, Kiel 24143, Germany
[5] IMED-Lab, Faculty of Science and Technology, Cadi Ayyad University (UCA), BP549, Marrakesh, Morocco
[6] Mining Environment and Circular Economy program (EMEC), Mohammed VI Polytechnic University (UM6P), Lot 660. Hay Moulay Rachid, 43150, Ben Guerir, Morocco
[7] Materials Science, Energy and Nano-engineering Department, Mohammed VI Polytechnic University (UM6P), Lot 660, Hay Moulay Rachid, 43150 Benguerir, Morocco
[8] Department of Physics, University Koblenz-Landau, 56070, Koblenz, Germany

Layered pigments used in coatings are becoming very attractive due to the improvement of the coating's barrier properties. The present investigation adopted long-term electrochemical approach to study the mechanisms of a new class of anti-corrosive coatings, based on alkyd with a novel hybrid phosphate pigment 6-amino hexanoic acid (6-AHA) intercalated in layered aluminum di-hydrogen tripolyphosphate (ATP-6-AHA) at 5.0 wt.% and applied on low carbon steel. The current study revealed superior corrosion protection of ATP-6-AHA coating on carbon steel with a polarization resistance of 1.3 108 Ohm×cm2 after three weeks immersed in a 3.5 wt.% NaCl solution, using electrochemical impedance spectroscopy (EIS). The surface roughness and adhesion of coated samples were evaluated using pull of test and laser scanning microscope. X-ray diffraction (XRD), Scanning electron microscope (SEM) were employed to assess the corrosion protection of ATP-6-AHA alkyd coating. Results revealed a protective film on steel surface comprising iron phosphate.

Sciforum-060880: Characterization, Surface Modification and Performance of an Additive Manufactured Al alloy

Esther López[1], Marta Mohedano[1], Hugo Mora-Sánchez[2], Rubén del Olmo[3], Marcos Díez[4], Endzhe Matykina[1], Raúl Arrabal[1]

[1] Departamento de Ingeniería Química y de Materiales, Facultad de Ciencias Químicas, Universidad Complutense, 28040, Madrid, España
[2] CIDETEC, Basque Research and Technology Alliance (BRTA). Po Miramón 196, 20014 Donostia-San Sebastian, Spain.
[3] Institute of Optoelectronics, Military University of Technology, 2 Kaliskiego Str., 00-908 Warsaw, Poland
[4] Advanced Manufacturing Processes Unit, AIMEN Technology Centre, 36418, O Porriño, Spain

The present work reports on the characterization, surface modification, and performance of additive manufactured (AM) 5083 alloy in comparison with its counterpart manufactured by conventional wrought route. The AM aluminium alloy was manufactured via wire-laser additive manufacturing (w-LAM), which produces an atypical microstructure that modifies both physical and chemical properties. Microstructures of the materials were analyzed using optical and scanning electron microscopy, X-ray diffraction and energy dispersive X-ray spectroscopy. The surface modification of the materials based on anodizing was also explored. The corrosion performance of the materials was evaluated using electrochemical techniques (Potentiodynamic polarization and Electrochemical Impedance Spectroscopy) in sodium chloride solutions. Results were compared with those obtained for conventional 5083 wrought alloy.

Sciforum-061018: Corrosion protection of AlSi7Mg0.3 using zirconium conversion treatment and polyacrylate siloxane-silica sol-gel coating

Peter Rodič, Veronika Bračič, Barbara Kapun, Ingrid Milošev

[1] Jožef Stefan Institute, Jamova cesta 39, 1000 Ljubljana, Slovenia

Cast aluminium alloy AlSi7Mg0.3 is a lightweight metal commonly present in the transportation industry. Due to the presence of alloying elements and intermetallic particles, aluminium alloys are susceptible to localised types of corrosion. Therefore, developing an environmentally acceptable corrosion protection system that can protect the substrate is desirable.
Adequate corrosion protection can be achieved with chromate conversion coatings, but such surface treatment may contain hexavalent chromium, which has been limited due to its harmful effect on humans and the environment. As an alternative, zirconium conversion coatings (ZrCC) as a pretreatment for aluminium surfaces [1] and polyacrylate siloxane-silica sol-gel coating [2] and their multilayer coating system present a novel corrosion protective coating system.
In the current study, the corrosion performance of ZrCC, polyacrylate siloxane-silica sol-gel coating and their multilayer system were studied. The ZrCC was formed in three steps (degreasing, desmutting, and passivation) using commercial reagents distributed by SurTec. The synthesis of hybrid sol-gel coating included inorganic compound: tetraethyl orthosilicate and organic compounds: 2-ethylhexyl acrylate and 3-(trimethoxysilyl)propyl methacrylate. The synthesis of the sol-gel coating was evaluated at various stages using real-time infrared spectroscopy. The corrosion characterisation was performed in 0.1 M NaCl using electrochemical impedance spectroscopy and salt spray test according to the ASTM B117 standard.
The results indicate that ZrCC and hybrid sol-gel coating form a continuous, smooth multilayer system, only a few micrometres thick. The multilayer ZrCC/sol-gel system provides more efficient long-term corrosion protection than individual ZrCC and sol-gel layers.
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Sciforum-060666: Effect of Sealing Temperature on the Corrosion Resistance and Mechanical Properties of Sulphuric Acid Anodized 6060 Aluminium Alloy.

Stanley Ofoegbu, Fábio A. O. Fernandes, Igor Bdikin, António B. Pereira

[1] Centre for Mechanical Technology and Automation (TEMA), Department of Mechanical Engineering, University of Aveiro, Campus Universitário de Santiago 3810-193 Aveiro, Portugal.

Energy reduction in industrial-scale aluminium anodization can be achieved by carrying out the sealing process step at lower temperatures (98 °C). In this work, sulphuric-acid-anodized AA6060 aluminium alloy samples were hydrothermally sealed for 30 minutes in de-ionised water at varying temperatures—50 °C, 60 °C, 70 °C, 80 °C, 90 °C, and 98 °C, respectively—and the effect of the sealing temperature on both the mechanical properties and corrosion resistance of the coating was determined. A simple electrochemical method for evaluating the barrier properties (corrosion resistance) of sealed and partially sealed anodized aluminium samples is demonstrated.1

Sciforum-060879: Functionalized hybrid PEO/Sol-gel Coatings for corrosion protection of Mg alloys

Borja Pillado[1], Marie-Georges Olivier[2], Isis Tournay-Dufrenne[2], Endzhe Matykina[1], Raúl Arrabal[1], Marta Mohedano[1]

[1] Departamento de Ingeniería Química y de Materiales, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, 28040 Madrid, Spain
[2] Materials Science Department, Université de Mons, 7000, Mons, Belgium

Inhibitor-containing systems based on plasma electrolytic oxidation (PEO) coatings with a sol-gel top layer were developed on AZ31 Mg alloy to improve its corrosion resistance. The 8-Hydroxiquinoline (HQ) inhibitor species were incorporated into the hybrid PEO/sol-gel system following two strategies: i) post-treatment of the PEO layer by immersion in an inhibitor containing solution or ii) loading of the inhibitor into the sol-gel precursor. Characterization was carried out by scanning electron microscope (SEM), X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), ultraviolet-visible spectroscopy (UV-vis), and water drop contact angle measurements. The rheological behaviour of the sol-gel solutions was determined by measurement of the flow curves using a double-gap cylinder configuration. The corrosion process was studied in saline solution using electrochemical impedance spectroscopy (EIS) on unscratched samples and immersion tests with scratched specimens. Findings revealed successful incorporation of the inhibitor for both loading strategies. Regardless of the loading strategy, the systems containing HQ species revealed the best long-term corrosion performance.

Sciforum-061015: Hydrotalcite modified coatings for corrosion protection of steel and Zn sacrificial layers

Duong Thuy Nguyen[1], Thuy Thu Pham[2], Justine Rodriguez[2], Hang Thi Xuan To[1], Marjorie Olivier[2]

[1] Institute of Tropical Technology
[2] Université de Mons

Steel is recognized for its good mechanical properties but also for being prone to corrosion leading to the formation of red voluminous products. The most used protection systems consist in the application of a zinc sacrificial coating and a conversion layer as phosphatizing or chromate-based ones which are known for toxicity or slurry production. Hydrotalcites (HT) are a class of anionic and basic clays made of a double layer hydroxide structure. Due to their lamellar morphology and negative global charge, these clays can be used for the intercalation of anionic species, such as carbonate, chloride, or inhibitive ones. The synthesis is performed by using low cost and environmentally friendly compounds. In this talk, different uses of these HT clays for the corrosion protection will be presented: 1) incorporation of hydrotalcite powders modified by different inhibitive species in an epoxy coating for the corrosion protection of steel and Zn sacrificial layer, 2) in situ growth of hydrotalcites on Zn sacrificial layers. Parameters, such as the role of the intercalated organic inhibitive species, their release, the nature of the substrate, and the corrosion protection mechanisms, will be discussed. Characterization was carried out by scanning electron microscope (SEM), X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), zêta potential measurement, TOC analysis, and ultraviolet-visible spectroscopy (UV-vis). The corrosion mechanisms were studied in saline solution using electrochemical impedance spectroscopy (EIS) and polarization measurements.

Sciforum-060826: Synthesis and properties of titanium carbide incorporated nickel phosphorus-based nanocomposite coatings.

Osama Fayyaz[1], R. A. Shakoor[1], Khuram Shahzad[2], Ahmed Bahgat Radwan[1], M. Adeel Umer[2]

[1] Center for Advanced Materials (CAM), Qatar University, 2713 Doha, Qatar.
[2] School of Chemical and Materials Engineering (SCME), NUST, 44000, Islamabad, Pakistan

Ni-P coatings have widely been reported to possess superior corrosion resistance ability and adequate mechanical properties. In order to further improve its performance nanospecies of titanium carbide (TiC) with various concentrations were pulse electrodeposited on high strength low alloy steel coupons (HSLA). The coatings were synthesized from modified Watts chemical bath and optimized pulse parameters to obtain nanocomposite coatings with minimum defects. Successful incorporation of TiC nanospecies has positively impacted the morphology, mechanical and anti-corrosive properties of nanocomposite coating as compared to simple Ni-P coating. The study encompasses physico-chemical behavior of as deposited coating through XPS, XRD, SEM, EDS and AFM. Moreover, mechanical characteristics of nanocomposite coatings were studied through Vickers microhardness tester, nanoindentation and ball on disk method of tribometry. It also analyses the wear track through profilometric measurements and magnified micrographs to elucidate the wear mechanism of the coatings. Furthermore, corrosion behavior was studied through potentiodynamic polarization and insights into the corrosion resistant mechanism is proposed through electrochemical impedance spectroscopic analysis.

Sciforum-060687: The effect of ALD oxides thin films on the electrochemical properties of the sputtered Al-Zr coatings

Elias KAADY[1, 2], Akram ALHUSSEIN[1], Mikhael BECHELANY[3], Roland HABCHI[2]

[1] UR LASMIS, Université de Technologie de Troyes (UTT), Pôle Technologique Sud-Champagne, 52800, Nogent, France
[2] EC2M, Faculty of Sciences, Campus Pierre Gemayel, Lebanese University (UL), Fanar, 90656, Lebanon
[3] Institut Européen des Membranes, IEM–UMR 5635, Université de Montpellier, ENSCM, CNRS, Montpellier, France.

Supersaturated solid solution Al–Zr film deposited by DC magnetron sputtering is used to provide sacrificial corrosion resistance to steels [1-2]. Recently, research has been focused on developing duplex coatings deposited alternately by both physical vapor deposition PVD and atomic layer deposition ALD techniques [3]. ALD oxide thin films were inserted into the Al-Zr coating. The main aim of the present work is to evaluate the effect of combined PVD and ALD thin films. This study shows a systematic comparison between different architectures and highlights the advantages and limits of each configuration. The morphology of the films is investigated by observing SEM images, the preferred orientation growth by XRD, and the topography by atomic force microscopy. The wettability behavior is determined using the contact angle technique. The nanoindentation measurements confirmed the enhancement in the hardness of the studied coatings. The electrochemical properties and corrosion behavior of these films were studied after being immersed in 3.5 wt% NaCl solution.

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Abstracts

Session 5: Corrosion in New Materials (HEA, CCA, TWIP/TRIP, AM, PM)

Sciforum-061826: Corrosion of Lightweight Concentrated Alloys: Roles of the Passivating vs. Non-Passivating Elements

Wenjun Cai[1]

[1] Materials Science and Engineering, Virginia Tech

To simultaneously enhance corrosion and strength, it is desirable to form lightweight concentrated alloys (LCAs), where the high solute concentrations (typically above ~ 5 at%) in the solid solution strengthen the material without compromising corrosion resistance. Examples of such LCAs include Al-based supersaturated solid solutions, metallic glasses, and emerging lightweight medium- to high-entropy alloys. In this talk, I will discuss our recent study on the corrosion and passivation behavior of Al-Mn-Mo LCAs, investigated by experiments and atomistic simulations. The pitting potential of Al-Mn-Mo was found to increase with Mo concentration, while the passive film thickness depended on the total alloy concentration. The oxidation of the passivating element vs. the selective dissolution of the non-passivating elements was found to govern the compactness and defect density of the passive layer. Finally, the experimental observations coupled with reactive force-field molecular dynamics simulations suggested that Mo slightly increased the Al-Al bond distance in the metal, resulting in a more compact passive film and higher corrosion resistance in Al80Mn8Mo12 than that of Al80Mn20.

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Session 6: Corrosion in the Energy Sector (Renewable and Nuclear)

Sciforum-057802: Corrosion Prediction Models in the Reinforcement of Concrete Structures of Offshore Wind Farms

Kerman Vázquez[1], Raúl Rodríguez[2], María Dolores Esteban[2]

[1] PhD Student
[2] Department of Civil Engineering, Universidad Europea de Madrid

Offshore wind will be one of the key technologies for achieving decarbonization targets over the next three decades. The growth of offshore wind farms (OWFs) is expected to be significant and to ensure their sustainable development it will be necessary to reduce its overall production costs, including the cost of maintenance activities during the service life of the WF. The foundation has become structurally more important in recent years due to the increasing size of wind turbines. Concrete is becoming increasingly important in the offshore wind industry as a main material, and as a constituent material in some secondary elements of current foundation typologies. With concrete structures, particular attention must be paid to corrosion of embedded steel especially in marine environments, as poor maintenance management can result in significant economic and structural safety consequences.
A tool has been developed to estimate the diameter loss in the reinforcement of concrete structures in OWFs and the subsequent loss of structural capacity, based on a systematic analysis of prevalent corrosion prediction models. For its validation, the tool methodology is applied to 32 real cases to evaluate the difference between the calculated and the real diameter loss. It has been demonstrated that the results obtained by using a combination between the chloride diffusion model of the Spanish code on structural concrete (EHE-08) for calculating the corrosion initiation period and the corrosion rate model of Li (2004) for calculating the corrosion rate guarantees favourable diameter loss prediction results.
Finally, to easily predict the loss of diameter as a function of time, a tool has been developed to estimate the loss of strength capacity of various structural elements as a function of time. This provides OWF operators with a valuable management tool for the planning of maintenance strategies and cost optimisation.

Sciforum-060986: Effects of pH and zwavelzure amoniak (ZA) fertilizer on the corrosion resistance of X60 steel in soils

Miftahul Jannah[1], Asep Ridwan Setiawan[1], Aditianto Ramelan[1]

[1] Institut Teknologi Bandung

Deterioration of buried steel pipelines due to corrosive soil environment is an inevitable issue in many countries, including Indonesia. Its tropical climate with heavy rainfall makes most of the soil to be acidic. In addition, as an agricultural country, the use of inorganic fertilizers in Indonesia is very high which can be corrosive to steel. One of the widely used fertilizers is *zwavelzure ammoniak* (ZA) which contains nitrogen and sulfate. This type of fertilizer can decompose or react to produce aggressive compounds such as ammonia (NH_3) and hydrogen sulfide (H_2S).
There have been many previous studies on the influence of soil pH on the corrosion resistance of steel pipelines in soil. However, only a few studies have examined the effect of fertilizers or the combined effect of pH and fertilizers, especially in Indonesian territory. Therefore, in this study, the corrosion behavior of X60 steel was investigated in Indonesian soil under the combined action of ZA fertilizer and soil pH. The corrosion kinetics were studied by weight loss, potentiodynamic polarization, and electrochemical impedance spectroscopy (EIS) measurements. It showed that the corrosion rate decreased with increasing pH in each concentration of ZA. Meanwhile, the effect of ZA fertilizer was significant only in soil with a pH of 7, in which the corrosion rate was proportional to ZA concentration. Overall, the highest corrosion rate was in the soil with the lowest pH and the highest ZA concentration, and vice versa for the lowest corrosion rate. It could be related to ZA behavior in lower the soil pH by removing alkaline ions like calcium from soil particles and replacing them with hydrogen ions. It made the corrosion even greater at lower pH.

Sciforum-060866: Evaluation of long exposure behavior of IN617 under high temperature and high-pressure air and steam environments

RISHIKESH K V[1], Satyanaryanan Seshadri[1], Subramanya Sarma V[1], Kamaraj M[1]

[1] IIT MADRAS

India's growing power demands and emission norms require more efficient coal-based power plants. The shifting of power plants from sub critical to ultra-supercritical (USC) steam conditions can improve efficiency by 12% and reduce CO_2 emissions by 35%. The candidate materials, such as Haynes 230, Super304H, and IN 617, are generally tested worldwide under either high temperature air (or) atmospheric pressure steam environments. There is a need to develop and qualify materials under ultra-supercritical steam conditions with high temperatures and high pressures in lab scale in India.
The sample materials were exposed to high temperatures of 700^{o}C in air and high pressure steam at 700^{o}C /243 bar for 1000 hours in as received and grain boundary enhanced condition. Grain boundary enhancement included optimization of a thermo-mechanical process involving cold rolling and annealing on samples. The effect of air and steam oxidation on IN 617, a Nickel based candidate super alloys was analyzed. Steam oxidation was performed on a custom built PARR 4650 series autoclave and oxidized samples were characterized under Scanning electron microscopy to evaluate the scales on the corroded coupons.
The grain boundary engineered material performed better than as received samples. IN 617 overall fared better under both air and steam conditions with very less weight gains.

Sciforum-060968: Experimental characterization of aluminum exposed to acid mine drainage corrosion

Julio José Caparrós Mancera[1], Ángel Mariano Rodríguez-Pérez[1], José Antonio Hernández Torres[1]

[1] University of Huelva

Aluminum is a widely used material in different activities related to mining. In this work, the effect of corrosion is analyzed. In addition, it is characterized how it affects the mechanical properties of aluminum. Acid mine drainage (AMD) is caused by the leaching of metal sulfides and pyrite. Furthermore, this is one of the main issues to be faced by mining exploitation. In addition to having critical effects, at an ecological level, on the environment where it occurs, its permanence over time can last for centuries. Moreover, once it appears it is virtually impossible to remove it, due to the high cost of technology. This situation motivates to analyze the behavior of aluminum coping with this environmental agent. To this end, a study focused on the corrosion incurred as a result of the exposure of aluminum to acid mine drainage and the subsequent mechanical tests is carried out. The study is based on the artificial exposure of metal test tubes to acid mine drainage by submerging them in highly concentrated rivers flow. Next, the test tubes undergo fatigue tests with the aim to characterize mechanical properties, developing the S-N curve. In this way, a specific and experimental analysis of the effects of corrosion on aluminum, in the context of acid mine drainage, is provided.

Sciforum-060890: Compatibility of different metallic materials and a novel salt hydrate phase change material slurry as secondary refrigerant for building air conditioning

Wenye Lin[1, 2], Stefan Gschwander[1]

[1] Fraunhofer Institute for Solar Energy Systems ISE, Freiburg 79110, Germany
[2] Sustainable Buildings Research Centre (SBRC), University of Wollongong, NSW 2019, Australia.

The increasingly severe climate change over the last few decades have aroused global concern and stimulated the development and deployment of energy-efficient technologies. Phase change material (PCM) slurries which can be used as thermal energy storage media and heat transfer fluid simultaneously, are among these sustainable technologies and have been attracting attention in many fields. In the building sector, they have been recognized as an effective alternative to serve as secondary refrigerant for energy management and transportation in building air conditioning systems. Among various PCM slurries, slat hydrate PCM slurries present many advantages, such as high cost-effectiveness, easy preparation and adjustable phase change temperature, etc., however, a barrier impeding the widespread application is their corrosive effect on metals. This study investigated the compatibility of a novel calcium chloride hexa-hydrate ($CaCl_2 \cdot 6H_2O$) based salt hydrate PCM slurry and different metallic materials. A dynamic immersion test was designed and implemented to reveal the carrion behaviors of seven metals typically used in air conditioning systems, including carbon steel, black steel, aluminum, stainless steel 304 and 316, cupper, and brass in the salt hydrate PCM slurries. The mass losses of metallic samples were measured according to American Society for Testing and Materials (ASTM) standards, and the phase change behaviors of the pre- and post-corrosion salt hydrate PCM slurry were comparatively characterized, to understand the effect of corrosion on the metals and the PCM slurry, respectively. The results showed that stainless steels and aluminum can be recommended for long term service, while caution needs to be taken when using the steels and cupper alloys. It was also found that the phase change characteristics of pre- and post-corrosion salt hydrate PCM slurry were identical, indicating a neglectable influence of corrosion on the function of slurry.

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Session 7: Corrosion in Biomedical Implants

Sciforum-062497: Corroding Zinc Scaffolds: Using Art of Metallurgy to Combat Vascular Diseases

Jaroslaw Drelich[1]

[1] Department of Materials Science and Engineering, Michigan Technological University, Houghton, MI 49931, USA

Coronary and peripheral artery diseases, such as atherosclerosis, are caused by the narrowing of the blood vessels with either fat or calcium deposits and are detrimental to the continuity of blood flow. Stents are commonly used in conjunction with angioplasty procedures to increase the diameter of the plagued vessel and restore the blood circulation. Bare metal stents provide mechanical support as vessel scaffolding and polymer-coated drug-eluting stents provide additional molecular therapy, but are needed only for a short time during reendothelialization and arterial wall stabilization. This short-term benefit can be overshadowed by long-term complications such as unfeasibility of second scaffolding in stented arteries of growing children and teenagers, chronic inflammation, late-stage thrombosis, restenosis, to name a few. To combat the long-term side effects associated with present generation of drug-eluting stents, a new generation of bioresorbable stents has been introduced. Stents made of bioresorbable materials are corroded and absorbed by the body after completing their task as vascular scaffolding, allowing the stented arteries to restore their normal function. The concept is achieved by engineering stents that retain mechanical properties and integrity for at least 4–6 months before being broken down, metabolized, and harmlessly excreted by the body, leaving the administrated vessel with a healthy endothelium, normal vasomotion and free of implant. In this presentation, the author will briefly review the status of development of zinc-based bioresorbable materials for stenting applications, their mechanical properties and behavior in vascular environment, in comparison to other metallic candidates, such as magnesium, iron, and molybdenum. Emphasis will be given to challenges in the formulation of high strength zinc materials that are biocompatible in the vascular environment. Type of corrosion products produced during the in vivo degradation will be reviewed as well.

Sciforum-060945: Developing Biodegradable Zn-Ca-Cu alloys for Wound Closure Applications

Jeffrey Venezuela[1], Nan Yang[1], Nagasivamuni Balasubramani[2], Helle Bielefeldt-Ohmann[3], Rachel Allavena[4], Sharifah Almathami[1], Matthew Simon Dargusch[1]

[1] School of Mechanical and Mining Engineering, EAIT, The University of Queensland
[2] Lightweight Materials and Manufacturing Research Laboratory, Ohio State University
[3] School of Chemistry & Molecular Biosciences, The University of Queensland
[4] School of Veterinary Science, The University of Queensland

A biodegradable Zn-1.0Cu-0.5Ca alloy was developed and has shown promise for wound closure applications. Ultrasonic treatment was used to refine and redistribute $CaZn_{13}$ particles in the cast alloy, which led to marked improvements in formability and post-deformation processing strength. The corrodibility of the alloy in a simulated physiological improvement was confirmed using polarization and immersion tests. The refined microstructure improved corrosion homogeneity, resulting in enhanced mechanical strength retention after prolonged exposure to physiological fluids. Cytotoxicity tests in human umbilical vein endothelial cell (HUVEC) and murine fibroblast cell (L929) indicated the alloy's good biocompatibility. Early attempts to fabricate a biodegradable staple from the rolled alloy will be discussed.

Sciforum-059234: Effect of deposition temperature on properties of hydroxyapatite coatings deposited on biodegradable AZ31B alloy

Alina Vladescu[1], Gianfranco Palumbo[2], Giuseppina Ambrogio[3], Diana M Vranceanu[4], Anca C Parau[5], Pasquale Guglielmi[6], Angela Cusanno[6], Mihaela Dinu[7], Giuseppe Serratore[3], Cosmin M Cotrut[4]

[1] National Institute for Optoelectronics, Department for Advanced Surface Processing and Analysis by Vacuum Technologies, 409 Atomistilor St., Magurele, RO77125, Romania
[2] Department of Mechanics, Mathematics and Management, Politecnico di Bari, Via Orabona4, 70126, Bari, Italy
[3] Department of Mechanical, Energy and Management Engineering - University of Calabria, P. Bucci, 87036 Rende (CS), Italy
[4] University Politehnica of Bucharest, 313 Spl. Independentei, Bucharest, RO60042, Romania
[5] National Institute of Research and Development for Optoelectronics - INOE 2000, Department for Advanced Surface Processing and Analysis by Vacuum Technologies, 409 Atomistilor St., Magurele, RO77125, Romania
[6] Department of Mechanics, Mathematics and Management, Politecnico di Bari, Via Orabona4, 70126, Bari, Italy
[7] National Institute of Research and Development for Optoelectronics - INOE 2000, 409 Atomistilor St., R077125, Magurele, Romania

The deterioration rate of Mg alloys is a challenging topic because these alloys exhibited a speedy degradation rate in the human body (Simulated Body Fluid, SBF). Many researchers try to find a solution for controlling Mg alloys degradation rate into solution found in SBF. The goal of the current paper is to coat AZ31B alloy by hydroxyapatite (HAp) in order to see its effect on the degradation rate. HAp coatings were obtained by RF magnetron sputtering method, by varying the deposition temperature from the room one to 400°C. The temperature could not be higher in order to avoid too large structural and mechanical changes. The experimental studies revealed that the grain size of the AZ31B alloy increased more than 100% when the deposition temperature was increased. The hardness of AZ31B alloy was decreased up to 15% by increasing the deposition temperature. Regarding the coatings, all of the HAp coatings increased the degradation rate of AZ31B, whatever was the deposition temperature. By comparing the coatings, those obtained at 200 °C proved to be the best solution for improving the corrosion of AZ31B alloy in SBF at 37°C since the protection to the corrosive attack of the SBF was about 97.3%. By increasing the deposition temperature to values larger than 200 °C, both mechanical and anticorrosion properties of the AZ31B-HAp coating are lost.
We acknowledge the support of the Romanian Ministry of Education and Research, CNCS - UEFISCDI, project ERANET-M-ISIDE-1, no. 171/2020 (INOE partner) and ERANET-M-ISIDE-2 no. 172/2020 (UPB partner), within PNCDI III.

Sciforum-059218: The comparability of in vitro and in vivo experiments for degradable Mg-implants

Regine Willumeit-Römer[1], Berit Zeller-Plumhoff[1], Christian Cyron[2]

[1] Helmholtz-Centre Hereon, Institute for Metallic Biomaterials, Max-Planck-Str. 1, 21502 Geesthacht
[2] Helmholtz-Centre Hereon, Institute of Materials Systems Modeling, Max-Planck-Str. 1, 21502 Geesthacht, Germany

Thousands of patients have already successfully been treated with Mg implants, and the number of approved products increases. Yet, we still have not reached a full understanding of all processes during the degradation of such implants and regeneration of the surrounding tissue. In vitro studies with sufficient spatial, temporal, and chemical resolution are challenging, and longitudinal in vivo monitoring with equally good resolution is typically even impossible. Therefore, we are aiming at the development of a Digital Twin for in silico studies. To calibrate this digital twin, we use not only reliable electrochemical data but also in vitro and in vivo imaging data with highest resolution (e.g., synchrotron radiation-based micro computed micro- and nano-tomography or transmission electron microscopy). These data enabled us to determine the degradation rates for Mg-xGd implant materials (x=2, 5, 10 wt. %). The data showed some unexpected structural features at the nanoscale within the degradation layer which could explain the differences in degradation rate in different media. In addition, different modelling approaches were used to describe the observations. In summary, we have the first module of a Digital Twin for the degradation at hand which will be coupled with a model of the tissue regeneration.

Sciforum-062871: The corrosion behavior of pure Zn in simulated body fluids

Yufeng Zheng[1]

[1] School of Materials Science and Engineering, Peking University, Beijing 100871, China

Background: The biodegradation of implants in physiological environment can be systematically affected by a host of factors, including inorganic ions, organic molecules, cells, pH, mechanical stimulus, and so on. The corrosion behavior of pure Zn was studied in the present work.
Methods: Hanks' solution, simulated body fluid (SBF), Dulbecco's modified Eagles' medium (DMEM), and DMEM with 10% Fetal Bovine Serum (FBS) were used as corrosion mediums.
Results: It turned out that the chemical composition of simulated body fluids can significantly affect the corrosion behavior of Zn, changing the corrosion rate and the corrosion product. The discrepancies of inorganic ions and organic components among four electrolytes played the fundamental role in the corrosion of pure Zn and contributed to the distinct corrosion processes consequently. Insoluble salts and organic components in DMEM can retard the corrosion of Zn, while the rapid protein adsorption on the surface altered the corrosion mechanism of Zn and greatly exacerbated the localized corrosion. The solution pH can remarkably affect the formation of corrosion product on pure Zn immersed in NaCl solution and SBF and can be effectively adjusted by three buffer systems (Tris-HCl, HEPES, and NaHCO3/CO2). The influence of H2O2 on the corrosion rate, corrosion product formation and corrosion morphology changed with its concentration, and greatly differed between PBS and Hank's solution. Meanwhile, Fenton reactions taking place in Hank's solution can also affect the degradation of pure Zn.
Conclusions: The solution pH, inorganic ions and organic components were recommended for the deeper investigation to further understand the corrosion of Zn. Tris-HCl or NaHCO3/CO2 buffered SBF yield the best replication for in vitro Zn characterization among these electrolytes. H2O2 can raise the corrosion potential of Zn and change the current density. Based on results, a reasonable proposal is thus put forward that the corrosion of Zn as the biological con sequence should be ta ken into consideration in evaluating the biodegradable metals.

Sciforum-060853: The prospect of biodegradable metallic mesh for pelvic floor reconstruction: dynamic behaviour point of view

zahrina mardina[1], Jeffrey Venezuela[1], Christopher Maher[1, 2], Zhiming Shi[1], Matthew Simon Dargusch[1], Andrej Atrens[1]

[1] The University of Queensland
[2] Department Urologynaecology, Royal Brisbane Women Hospital (RBWH)

Pelvic organ prolapse (POP) refers to the herniation of organs in the pelvic floor cavity, including bladder, rectum, uterus, and urethra. The weakening of the supporting muscles causes POP. The condition affects over half of the women population who have given birth. POP results in discomfort to chronic pain. In 25% of surgical procedures for POP opted for polymer-based surgical mesh, referred to as pelvic mesh. In 2013, the US food and drug administration (FDA) reclassified pelvic mesh into class III high-risk medical devices upon receiving 1503 complaints. The complaints included infection, erosion, exposure, and perforation. The problems classifications are (1) materials induced prolonged inflammation and (2) mechanical mismatch.
The factors influence meshes' mechanical properties are (1) the single yarn properties, (2) the textile architecture, such as weave or knit. The textile architecture contributes to meshes' flexibility. The initial stiffness assessment for various polymer-based meshes showed a good stiffness match with pelvic floor tissues. However, the pelvic mesh is implanted in a mechanically complex pelvic cavity. The mesh is sutured and needs to suspend the dynamically moving pelvic organs.
The problem with polymer-based meshes might be its tendency to change over time, referred to as dynamic behaviour. The underlying mechanical issues might be (1) strain hardening, (2) creep, and (3) fatigue failure. A promising alternative material to the polymer mesh might be biodegradable metals based on magnesium (Mg), zinc (Zn), and iron (Fe). Biodegradable metallic meshes offer some advantages, such as: (1) safely degrades after tissue healing is completed, reduces prolonged inflammation; (2) higher melting temperature for a better creep resistance; (3) higher fatigue resistance; and (4) higher yield stress which reduces the possibility of strain hardening.

Abstracts

Session 8: Atmospheric Corrosion

Sciforum-063263: Infrared-spectroscopy-based techniques for studies of atmospheric corrosion and degradation of coated materials

Dan Persson[1], Nathalie Lebozec[2], Dominique Thierry[1, 2], Alexander Wärnheim[1], Camilla Edvinsson[1]

[1] Research Institutes of Sweden (RISE), Kista, Sweden
[2] Institut de la Corrosion / French Corrosion Institute, Brest, France

Industrial coating systems such as coil coatings and automotive coatings are used in very large amounts to provide surface protection and for their aesthetic properties. Usually, these systems consist of a pretreatment layer applied on metal substrate and several organic coating layers. For steel substrates, zinc or zinc-alloy metal coatings are employed to increase the corrosion resistance of coated steel. The durability of such coating systems is determined by several factors including the stability of the substrate coating interface and transport of water and ions through the coating to the interfacial region. Weathering degradation of the organic coating layers can decrease the barrier properties of the organic coating layers and facilitate the ingress of water and ions into the system. Here, different techniques based on infrared spectroscopy are used to study the corrosion and degradation processes of a coating system on steel. It is shown that techniques based on infrared spectroscopy, such as *in situ* infrared reflection absorption spectroscopy (IRRAS), FTIR focal plane array imaging (FPA), FTIR photoacoustic spectroscopy (PAS) and AFM/Nano-IR are useful for studying different aspects related to corrosion and degradation processes of coatings. The benefits and limitations of infrared-spectroscopy-based techniques are discussed.

Sciforum-060988: Atmospheric corrosion of dissimilar friction stir welded AA2017 and AA7075 in urban area of Indonesia

Firdausi Hasbi Zamrudi[1], Aditianto Ramelan[1], Asep Ridwan Setiawan[1]

[1] Institut Teknologi Bandung

Friction stir welding is a promising joining technique that offers safety, reproducibility, lower energy consumption, without shielding gas and consumables, and does not involve a solidification process. Nevertheless, the atmospheric corrosion behavior of dissimilar friction stir weldments in each zone has not been widely studied. In this research, the electrochemical properties of the parent metal, thermo-mechanical affected zone, and stir zone in AA2017/AA7075 dissimilar friction stir welded are observed using open circuit potential, potentiodynamic polarization, and electrochemical impedance spectroscopy. We also conducted 120 days urban atmospheric corrosion test and characterized the result by visual photography and scanning electron microscopy equipped with energy dispersive spectroscopy. As a result, electrochemical testing data showed that corrosion progressed more rapidly in the stir zone and thermo-mechanical affected zone compared with the parent metal near the weldment area. Moreover, the exposed sample stir zone also showed the most corrosion pits among the other region. This weldments corrosion susceptibility is mainly caused by galvanic interactions between the AA2017 rich zones and AA7075 rich zones.

Sciforum-059237: Influence of exposure conditions and particulate deposition on anodized aluminum corrosion

Isabel Rute Fontinha[1], Elsa Eustáquio[1]

[1] Laboratório Nacional de Engenharia Civil (LNEC)

Anodizing is commonly used for corrosion protection of aluminum and its alloys in the construction industry. The anodic aluminum oxide (AAO) coating has a high ability to prevent the development of extensive pitting corrosion in the aluminum substrate, particularly in marine sites, as it was observed during a 10 years' atmospheric corrosion study carried out in several marine and industrial sites. However, this study also evidenced that this coating can be highly affected by the deposition of particulate material in industrial polluted environments, sometimes, in an unexpected way. This study presents the atmospheric corrosion of the anodized aluminum exposed in two different chemical industrial complexes: a fertilizer production plant and a pulp and paper mill. Visual assessment of surface changes, pitting depth, and mass variation with exposure were determined to quantify the degradation suffered. Additionally, SEM/EDS analyses were carried out on the exposed surface. Based on the results obtained, the role played by the deposition of airborne particles present in those two environments in the type and level of damage observed is discussed. These deposits: roasted pyrite ash and phosphates, or wood chips and lime particles, have enhanced pitting corrosion or caused dissolution of the AAO coating, respectively.

Sciforum-060999: Study of Atmospheric Corrosion Characteristics of Magnesium Alloy AZ31B in Tropical Rural and Urban Environments

Jasmita Nur Azizah[1], Asep Ridwan Setiawan[1], Aditianto Ramelan[1]

[1] Bandung Institute of Technology

Magnesium Alloys are of considerable interest in auto lightweight applications in the future. In that application, it was widely used in the atmospheric environment, such as steering components. However, the detailed information about the corrosion behaviour of Magnesium Alloys in tropical atmospheric corrosion has not been studied widely. This study investigated atmospheric corrosion of exposed Magnesium Alloy AZ31B in tropical rural and urban environments under NaCl and Na_2SO_4. The thin film formed was analyzed to determine the stability of Magnesium Alloy AZ31B in exposure tests carried out for 1, 2, and 4 months. The observation was investigated by weight loss experiments, electrochemical measurements, and surface morphology analysis. The influence of environmental parameters was played an important role in the corrosion process, indicated by the presence of pits. As a result, electrochemical measurements showed that the atmospheric corrosion rate increased with the exposure time due to increased corrosion products. The electrochemical test results also showed that the corrosion rate increased when NaCl induced the Magnesium Alloy sample more than Na_2SO_4. It stimulated corrosion by encouraging the formation of a thin electrolyte layer, increasing conductivity, and decreasing the protective effect of the corrosion layer.

Abstracts

Session 9: Microbiologically influenced Corrosion

Sciforum-057359: The experimental and theoretical approaches to the valorization of some pyridotriazine derivatives in the inhibition of copper corrosion in nitric acid medium.

Houda SERRAR[1], Moussa Ouakki[1], Hassane LGAZ[2], Fouad Benhiba[3], Mouhsine Galai[3], Said Boukhris[1], Amina Hassikou[1], Abdelaziz Souizi[1], Hassan Oudda[3], Mohamed Ebn Touhami[3]

[1] Organic Chemistry, Catalysis and Environment, Faculty of Science, Tofail, 14000 Kenitra, Morocco.
[2] Research Professor at Hanyang University-ERICA, Ansan, South Korea
[3] Advanced Materials and Process Engineering, Faculty of Sciences, Ibn Tofaïl University, PO Box 133, 14000, Kenitra, Morocco.

Copper is a multi-faceted metal. It is a trace element essential to life for all living organisms. As a metal, it has many properties that are essential to today's world. In addition, copper is known as a noble metal that provides corrosion resistance in most environments due to the formation of a passive protective film (oxide)[1,2].
In fact, deposited corrosion products have a negative effect on heat transfer. The heating efficiency of the equipment is reduced as a result of this effect, which necessitates periodic descaling and cleaning in acidic solutions.
In this regard, researchers have used corrosion inhibitors to protect copper against corrosion in different corrosive environments [4,5].
Therefore, in the present work, we were interested in evaluating the inhibitory efficiency of copper in nitric acid (2M) medium using three synthesized pyridotriazine-based derivatives, **1a**, **1b** and **1c**.
In this work, we studied the inhibition of copper corrosion in HNO_3 2M by organic compounds of the "pyridotriazine" type (**1a**, **1b** and **1c**). This study was carried out on the basis of experimental methods (polarization curves).
The study of the effects of concentration and temperature shows that the inhibitory efficiency increases with the concentration of the tested compounds. We found that pyridotriazine 1b is the best among the three tested compounds.
Analysis of the polarization curves allowed us to suggest that our inhibitors could be classified as mixed inhibitors with anodic predominance. The very negative values of **$\Delta G°_{ads}$** indicate that the adsorption of pyridotriazines **1a**, **1b** and **1c** occurs spontaneously on the copper surface.
The second part of this work shows that theoretical approaches, such as quantum chemical calculation and molecular dynamics simulation, have been used as powerful and rapid tools to help interpret the experimental results and clarify the corrosion inhibition mechanisms.

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Sciforum-060554: Evolution of microbial corrosion research from the previous century to the present

Pierangela Cristiani[1]

[1] Ricerca sul Sistema Energetico – RSE, Italy

Microbiological corrosion (MIC) was first observed at the beginning of the twentieth century. Still, it took about half a century to reach a rigorous (electrochemical) explanation on why sulfate-reducing bacteria induce surprisingly fast steel corrosion, despite the anaerobic conditions.

It took half a century more to state that bacteria also influence the cathodic corrosion reaction in aerobic conditions, ennobling the corrosion potential of stainless steel. Other than this fact, the second half-century produced a general agreement that biofilm plays a central role in changing the electrochemical condition on the metal surfaces, influencing and, in some cases, inhibiting the corrosion processes. Electrochemical probes able to monitor the biofilm in real-time for industrial sites were developed (in US and EU). The scientific discussion focalized on the involvement of enzymes in transferring electrons to the metal. Investigations of electroactive biofilm started worldwide, in-field and in labs, also thanks to EU financed programs.

In the meantime, innovative microscopy techniques documented the settlement of single bacteria on metal surfaces, while new spectroscopic and electrochemistry techniques individuated a clear relationship between corrosion products and biofilms, confirming their corrosive effects.

Studies at the laboratory level with single microbial species increased significantly in the new century after the amazing discovery that living organisms electrically communicate with conductive surfaces. Furthermore, next-generation sequencing of DNA and RNA tools allowed the discovery of many uncultivable bacteria and archaea responsible for MIC, in oil and gas especially.

The great interest in bioelectrochemical systems exploded after the 2008, contributing to crossing knowledge between electrochemists and microbiologists. Scientists of different backgrounds learned to strictly collaborate for understanding the fundamentals of microbial fuel cells and bioelectrolysis processes. Several microbial corrosionists participated in this process, making the "world of bioanode" match the "world of biocathode". MIC studies also benefited from the studies of bioanode but did not equally grow as microbial electrochemistry. It is time to fill the gap.

Sciforum-059750: Uptake of low-energy electrons from electrodes in Desulfovibrio vulgaris Hildenborough

Xiao Deng[1], Akihiro Okamoto[1], Anna Kaksonen[2]

[1] National Institute for Materials Science
[2] Commonwealth Scientific and Industrial Research Organisation

Sulfate-reducing bacteria (SRB) are the main cause of iron corrosion in many anaerobic environments. Multiple SRB strains have been shown to conduct extracellular electron uptake (EEU) from solid electron donors coupled with sulfate reduction. Given that EEU is much faster than diffusion-governed reactions between iron and SRB metabolites, such as hydrogen sulfide, EEU has been proposed to be a critical mechanism for the high corrosiveness of some SRB strains. *Desulfovibrio vulgaris* Hildenborough was recently shown to conduct EEU on electrodes with the aid of self-synthesized membrane bound FeS nanoparticles. However, the energetics of this process have not been elucidated, leaving its relevance to corrosion unclear. In the present study, whole-cell electrochemical measurements, single-cell activity analysis, and gene expression analysis were combined to study the energetics of the EEU process mediated via FeS nanoparticles. It was revealed that *D. vulgaris* was able to utilize low-energy electrons, even at -0.2 V (vs. SHE) for metabolism activation, suggesting an electron bifurcation mechanism for producing intracellular energy carriers with more negative redox potentials. The EEU onset potential was 100 mV more positive than reported values for EEU mediated via cell-surface redox proteins in other SRB strains. Therefore, FeS nanoparticles may provide more energetically favorable EEU pathways and promote iron corrosion at more positive potentials. Details of results and discussion will be presented at the conference.

Sciforum-060946: Isolation of a Bacterium from the Petroleum Environment and Evaluation of its Biocorrosion Impact on Steel

Fayza BOUCHAKOUR[1], El Hadj DRICHE[2]

[1] Hassiba Ben Bouali University of CHLEF ALGERIA, department of process engineering
[2] Hassiba Ben Bouali University of CHLEF ALGERIA

Internal pipeline corrosion is the leading cause of hydrocarbon pipeline leaks and ruptures, it is not only a source of waste of raw materials and energy, it can also lead to tragedies and ecological losses. Microbial corrosion of steel was studied by bacterial aerobic which was isolated from the injection water of the oil wells. Steel coupons were exposed to a culture of the bacterial strain for 7 and 15 days with a control group in an inoculated medium. The results of the present study suggest that the bacterial stump was responsible for the corrosion of the steel. These results were supported by the mass loss results and the electrochemical study

Sciforum-060555: Mechanisms for Microbially Enhanced Metal Corrosion Under Anaerobic Conditions

Derek R. Lovley[1, 2], Dandan Liang[2, 3], Dawn E. Holmes[2], Hai-Yan Tang[2], Dake Xu[4]

[1] Electrobiomaterials Institute, Key Laboratory for Anisotropy and Texture of Materials (Ministry of Education), Northeastern University, Shenyang 110819, China;
[2] Department of Microbiology, University of Massachusetts, Amherst, MA, USA
[3] State Key Laboratory of Urban Water Resource and Environment, School of Environment, Harbin Institute of Technology, Harbin, 150090, China
[4] Electrobiomaterials Institute, Key Laboratory for Anisotropy and Texture of Materials (Ministry of Education), Northeastern University, Shenyang 110819, China

Microbe-enhanced corrosion of iron-containing metals under anaerobic conditions has been known for some time, but until recently the proposed mechanisms that accelerate corrosion have not been rigorously evaluated. For example, the possibility that microbes can directly extract electrons from Fe(0) is commonly invoked, but evidence for this mechanism has typically been indirect. The possibility that H_2 was serving as an intermediary electron carrier during corrosion was not strictly excluded. Studies with strains of *Geobacter sulfurreducens* and *Geobacter metallireducens* that could not use H_2 as an electron donor reduced either nitrate, Fe(III), or fumarate with pure Fe(0) or stainless steel as the electron donor. Deletion of the genes for outer-surface *c*-type cytochromes known to be involved in extracellular electron exchange inhibited the corrosion. In a similar manner, *Methanosarcina acetivorans*, a methanogen that is incapable of H_2 utilization, reduced carbon dioxide to methane with pure Fe(0) or stainless steel as the electron donor. Deleting the gene for MmcA, an outer-surface multi-heme *c*-type cytochrome important for electron exchange with other extracellular donors/acceptors inhibited electron uptake. It was previously proposed that the sulfate-reducing microorganisms *Desulfovibrio ferrophilus* and *Desulfopila corrodens*, were capable of direct electron uptake because they corroded pure Fe(0) faster than some other sulfate reducers. However, recent studies found that *D. ferrophilus* and *Dp. corrodens* could not use stainless steel, an Fe(0) source that does not generate H_2 as an electron donor. These results suggest that, unlike the *Geobacter* and *Methanosarcina* species, neither of these sulfate reducers is capable of direct electron uptake. These results demonstrate the need to rigorously evaluate proposed corrosion mechanisms with the appropriate controls. The finding that outer-surface *c*-type cytochromes may be the electrical connections between Fe(0) and corrosion-enhancing microbes provides a tool for hunting for microbes capable of corrosion via direct electron uptake and suggests strategies for inhibiting their corrosive activities.

Sciforum-060556: Microbial Communities Associated with Carbon Steel Corrosion in Model Seawater Compensated Fuel Ballast Tanks

Kathleen E. Duncan[1], Mark A. Nanny[2], Lina E. Dominici[3], Irene A. Davidova[1], Brian H. Harriman[1], Joseph M. Suflita[1]

[1] Department of Microbiology & Plant Biology and OU Biocorrosion Center, University of Oklahoma, Norman, OK 73019, USA
[2] School of Civil Engineering and Environmental Science and OU Biocorrosion Center, University of Oklahoma, Norman, OK 73019, USA
[3] Centro de Investigación y Desarrollo en Tecnología de Pinturas (CIDEPINT), CICPBA-CONICET-UNLP, La Plata, Argentina

Duplicate rotating reactors containing carbon steel coupons were inoculated with seawater and either a petro- or Fischer-Tropsch F76 or a mix of both fuels. Controls included reactors without fuel and reactors containing sterilized seawater and fuels. After 389 days, one replicate of each treatment received either heat-sterilized or non-sterile sediments. Dissolved O_2, pH, oxidation-reduction potential (ORP), rates of sulfate reduction (SRA), and dissolved metal ions were monitored throughout the incubation. The reactors were disassembled after 730 days and the coupons, reactor fluids and sediment samples were obtained for sequencing analysis and assessed for evidence of corrosion.

Results: Dissolved O_2 was not detected in any reactor after day 11, and differences in pH, ORP, and corrosion rates (based on dissolved Fe and Mn) were observed by day 82. By these measures, reactors with fuel enhanced corrosion over seawater-amended controls. The addition of sediments caused pH to drop in the non-sterile seawater reactors, suggesting microbial activity was stimulated by exogenous organic carbon. SRA was generally insignificant, but transiently higher after sediment addition.

Microbial profiles from the seawater and sediment inocula were more diverse than samples from the reactors. In general, microbial profiles from coupons were similar in that all contained a high percentage of Deltaproteobacteria. *Desulfovibrio* dominated coupons from reactors without fuel, while coupons from reactors with fuel were more diverse and varied between replicates which received non-sterile rather than heat-treated sediments. The coupon communities from the 6 reactors that received non-sterile seawater and fuel were more similar to each other than to the fuel-unamended reactors, but the type of fuel did not determine the community profile. Compared to results from seawater-compensated fuel ballast tanks, a higher percentage of Deltaproteobacteria and lower percentage of aerobic hydrocarbon-degrading Gammaproteobacteria was typically observed in the reactors.

Sciforum-061025: Quorum-Sensing Driven Inhibitors for Mitigating Microbial Influenced Corrosion

Asma Lamin[1], Anna Kaksonen[2], Ivan Cole[3], Xiao-Bo Chen[4]

[1] RMIT University Melbourne Austaralia
[2] Commonwealth Scientific and Industrial Research Organisation (CSIRO), Land and Water, 147 Underwood Avenue, Floreat, WA 6014, Australia
[3] School of Engineering, RMIT University, Melbourne 3000, VIC, Australia
[4] School of Engineering, RMIT University, Melbourne 3000, VIC, Australia.

*Asma Lamin[a], Anna H. Kaksonen[b], Ivan Cole[a] and Xiao-Bo Chen[a],**
[a] School of Engineering, RMIT University, Melbourne 3000, VIC, Australia.
[b] Commonwealth Scientific and Industrial Research Organisation (CSIRO), Land and Water, 147 Underwood Avenue, Floreat, WA 6014, Australia

Abstract

Microbiologically influenced corrosion (MIC) is a process in which microorganisms initiate, facilitate, or accelerate the electrochemical corrosion reactions of metallic components. Several reports documented that MIC accounts for about 20 to 40% of the total cost of corrosion. Biofilm formation due to the presence of microorganisms on the surface of metal components is known to play a vital role in MIC, which can lead to severe consequences in various environmental and industrial settings. Quorum sensing (QS) system plays a major role in regulating biofilm formation and control the expression of some enzymes. QS is a communication mechanism between microorganisms that involves the regulation of gene expression as a response to the microbial cell density within an environment. This process is employed by both Gram-positive and Gram-negative bacteria to regulate different physiological functions. QS involves production, detection, and responses to signalling chemicals, known as auto-inducers. QS controls specific processes important for the microbial community, such as biofilm formation, virulence factor expression, production of secondary metabolites, and stress adaptation mechanisms. The use of QS inhibitors (QSIs) has been proposed as a possible solution to biofilm related challenges in many different applications. Although QSIs have demonstrated some strength in tackling biofouling, QSI-based strategies to control microbially influenced corrosion have not been thoroughly investigated. As such, our research aims to target the QS mechanisms as a strategy for mitigating MIC on metal surfaces in engineered systems.

Currently we are testing the corrosion inhibition efficiency of three different material that have been used as QSIs in literature. Tests are conducted on steel X65 in 0.1M NaCl using electrochemical techniques. Bacterial growth curve will be conducted to confirm that QSIs used in this study are not hindering the microbial growth. Later, steel samples will be immersed in bacterial culture with and without the QSIs, weight loss and different microscopic techniques will be used to study the bacterial behaviour and corrosion.

Sciforum-060942: The role of H2 on the acetogens influenced corrosion

Laura Munoz[1], Jo Philips[2]

[1] Biological and Chemical engineering, Aarhus University
[2] Biological and Chemical engineering , Aarhus University

The extracellular electron uptake from insoluble electron donors is a characteristic described for some microorganisms. Some acetogens can use Fe(0) as the only electron donor to reduce CO_2 into acetate. These acetogens participate in the biological acceleration of Fe(0) oxidation known as Microbial influenced corrosion, which is causing high economic costs. On the other hand, extracellular electron uptake by acetogens is also promising for biotechnological applications such as microbial electrosynthesis. However, the mechanisms used to obtain extracellular electrons by acetogenic bacteria are still unclear.
We evaluated the role of H_2 as an intermediate in the extracellular electron uptake. We hypothesize that strains with better adaptation to low H_2 partial pressures can easily use H_2 chemically produced on Fe(0) and promote cathodic H_2 evolution by a thermodynamical effect. There was limited and variable information about the H_2 consumption characteristics of acetogens.
The H_2 threshold (lowest partial pressure that allows H_2 consumption) and the H_2 consumption kinetic parameters of different acetogenic strains were evaluated. In addition, the influence of acetogens on the Fe(0) corrosion. The elucidation of the extracellular electron uptake mechanism of acetogens will allow a better understanding of microbial-induced corrosion and hopefully the development of new diagnostic tools and mitigation strategies.

Abstracts

Session 10. Corrosion of Magnesium Alloys

Sciforum-058526: Effects of deposition mechanism of corrosion products on corrosion rates of AZ91D and HP Mg under thin electrolyte layers (TEL)

Ningning Dan[1,2], Yao Yang[1,2], Tao Ying[1,2], Xiaoqin Zeng[1,2]

[1] National Engineering Research Center of Light Alloy Net Forming, Shanghai Jiao Tong University
[2] The State Key Lab of Metal Matrix Composites, Shanghai Jiao Tong University

Investigation on simulated atmospheric corrosion of Mg is a long-standing challenge. In this work, effects of deposition of corrosion products on corrosion rates and pseudo-passivation behavior of AZ91D and HP Mg under thin electrolyte layers (TEL) and in a bulk solution were investigated. Low corrosion rates and pseudo-passive behavior can be maintained over time under TEL, especially under extremely thin electrolytes (100-μm-thick and 200-μm-thick TEL). The results reveal that the deposition of corrosion products of Mg follows an activation-controlled growth mechanism. The surface of Mg is pseudo-passivated with good film integrity. Passivation behavior of AZ91D and HP Mg under TEL is promoted by the polarization resistance caused by limited mass transfer of corrosion products and cathodic polarization induced by the difficulty of H^+ to receive electrons and the H_2 to escape after formation under TEL. Passivation behavior under TEL is caused by the limited mass transfer of corrosion products composed of metal oxides, hydroxides, and carbonates.

Sciforum-063896: Corrosion in magnesium batteries: Current challenges and future perspectives

Parama Banerjee[1]

[1] Department of Chemical & Biological Engineering, Monash University, Australia

Owing to the abundance of magnesium in earth's crust, magnesium batteries have been attracting significant attention as a potential energy storage system for electric vehicles, grid storage as well as for internet of things (IOT). Even though magnesium anodes possess high theoretical capacity and energy density, the widespread practical application of magnesium batteries has been largely limited due to their high corrosion rate. In this talk, I am going to provide a critical review of the current challenges in magnesium batteries due to the high self-corrosion of magnesium anodes, as well as provide a brief overview of the recent development in strategies to suppress corrosion in these batteries..

Sciforum-059778: Microstructure of the Surface Corrosion Film on Biodegradable Mg Alloys in Simulated Body Fluids

Peng-Wei Chu[1], Cheng-Xun Yang[1], Chien-Wei Fan[1]

[1] Department of Engineering and System Science, National Tsing Hua University, Taiwan

Magnesium (Mg) and its alloys are promising biodegradable implants for orthopedic surgeries owing to their biocompatibility, similar mechanical properties to bones, and the ability to decompose in the human body. However, practical applications of biodegradable Mg implants are limited by the fast degradation rates of Mg alloys, leading to disruption of osseointegration and premature failure of the fixation. Therefore, understanding the corrosion behavior of Mg alloys in physiological environments is key to the development of Mg alloy implants. In this study, the corrosion morphology and microstructure of the surface corrosion film of two candidate biodegradable Mg alloys, WE43 (Mg-4 wt%Y-3 wt%Nd) and ZX21 (Mg-2 wt%Zn-1 wt%Ca), immersed in Hanks' balanced salt solution (HBSS) is characterized through *in situ* optical microscope (OM), scanning electron microscope (SEM), site-specific focused ion beam (FIB) milling, and cross-sectional transmission electron microscope (TEM) techniques. The surface corrosion films on both alloys in HBSS are mainly composed of O, Mg, P, and Ca, with a nanoporous noncrystalline structure. Nevertheless, the thickness of the surface corrosion film on WE43 is only about 80 to 100 nm, but the thickness of the film on ZX21 is about 300 to 400 nm with some scattered hollow corrosion products on top of the surface film. The corrosion behavior and electrochemical responses of the two alloys in HBSS will be discussed based on the corrosion morphology and the surface corrosion film microstructures.

Sciforum-060366: The in vitro corrosion studies of biodegradable magnesium-calcium alloy in different media

Andrey S. Gnedenkov[1], Valeriia S. Filonina[1], Sergey L. Sinebryukhov[1], Sergey V. Gnedenkov[1]

[1] Institute of Chemistry, Far Eastern Branch of the Russian Academy of Sciences, Vladivostok, Russia, 690022

Magnesium alloys, due to their unique properties, such as low specific weight and high strength characteristics, are promising materials for various fields of science and industry. Moreover, Mg and its alloys can be applied in implant surgery as biodegradable materials [1,2]. The corrosion behaviour of bioresorbable magnesium alloy Mg-0.8Ca was studied in physiological solutions (minimum essential medium (MEM) and 0.9 wt. % NaCl solution) using traditional (OCP, EIS, and PDP) and local scanning electrochemical (SVET, SIET with H^+-selective microelectrode) methods. Corrosion degradation rates of Mg specimens were evaluated using mass loss tests. The effect of media species, composition, and microstructure of the alloy on its electrochemical activity was established. The parameters of SVET and SIET measurements were optimized for *in vitro* studies of the biodegaradable Mg alloy. The mechanism of the material's corrosion degradation was revealed. The effect of secondary phases on the corrosion activity of the material was investigated by means of in situ analysis and SKPFM tests. The intensive corrosion rate of the Mg alloy is a result of the presence of anodic secondary phase, which creates a localized microgalvanic cell with α-matrix and facilitates the dissolution of Mg_2Ca compounds at the grain boundaries. The maximum electrochemical activity of the alloy was detected in the first 12 min of specimen immersion in MEM, followed by decrease of the corrosion intensity associated with material passivation. The complementary SEM-EDX, XPS, Raman microspectroscopy analysis showed the composition of the corrosion products, which included magnesium-and-carbonate substituted hydroxyapatite. The results indicated the low possibility of application of Mg-0.8Ca alloy without protection as a biodegradable implant in medicine [3].

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Sciforum-063019: Complexants as active modulators of Mg surface reactivity

Mikhail Zheludkevich[1]

[1] Institute of Surface Science, Helmholtz-Zentrum Hereon, Max-Planck Str. 1, 21502 Geesthacht, Germany

Magnesium and its alloys are among the lightest structural metallic materials and are also considered as promising materials for resorbable implants and energy storage. However, the high reactivity and the corrosion susceptibility of Mg in aqueous environments significantly limits the application range. However, the reactivity of the Mg surface can be controlled from both the metal and the electrolyte sides.

In this paper, the chelating agents able to form complexes with Mg cations and the cations of impurity elements are discussed as potential modulators of Mg surface reactivity.

The compounds capable of forming strong insoluble complexes with Mg^{2+} can confer an efficient inhibition of Mg dissolution blocking the surface by a dense layer of products. In turn, the modulators forming highly soluble complex can strongly affect formation of the corrosion products on the metal surface shifting the process towards faster dissolution of Mg, which can be relevant for the optimization of discharge properties of metallic Mg-based anodes. The talk will also address the strategies for selecting efficient modulators with targeted properties using Artificial Intelligence based approaches.

Sciforum-060559: Mg Corrosion: recent progress

Andrej Atrens[1]

[1] The University of Queensland, Materials Engineering Division, School of Mechanical & Mining Engineering, Centre for Advanced Materials Processing and Manufacturing (AMPAM), Brisbane, Qld 4072, Australia

Twenty years ago, stainless Mg was a research goal, and this goal remains relevant today. Most research has studied Mg corrosion in aqueous solutions, particularly in concentrated chloride solutions, because these are expected to provide information relevant to the corrosion of Mg in auto applications and for aerospace usage. It should, however, also be noted that Mg alloy corrosion in the atmosphere can be much less; for example, the atmospheric corrosion rate can be lower than the common aluminium alloys or steel. The main metallurgical factors controlling the corrosion of Mg alloys in aggressive chloride environments were clear: (i) corrosion acceleration by micro-galvanic corrosion by second phases, including Fe-rich phases, (ii) improved protectiveness of the surface film on the alpha–Mg matrix by alloying, and (iii) a decreased corrosion rate from microstructural refinement. These factors remain the metallurgical factors of importance for Mg corrosion. Over the last twenty years, a lot of research has been conducted with the aim of producing Mg alloys with low corrosion rates. The benchmark is the intrinsic corrosion rate of Mg of ~0.3 mm/y in a concentrated chloride solution and in a synthetic body fluid such as Hanks' solution. It should be mentioned that the corrosion mechanistic insights from the studies in concentrated chloride solutions are also relevant to the biocorrosion of Mg. This paper reviews the recent research on Mg alloy development and focusses on Mg alloys with low corrosion rates that are comparable to, or lower than, the benchmark of the intrinsic corrosion rate of high-purity Mg. Furthermore, recent research on the corrosion mechanism is reviewed. Experiments have shown that the enhanced catalytic mechanism does not explain the rate of anodic hydrogen production on anodic polarisation. In contrast, research has provided compelling evidence for the uni-positive Mg^{+} mechanism of Mg corrosion. Implications are discussed.

Abstracts

Session 11: Corrosion Inhibition

Sciforum-059751: Investigating the Microstructure and Corrosion of Additively Manufactured Steels with a View to Protection

[1]Anthony Hughes, [1]Majid Laleh, [1]Mike Y. Tan

[1] Deakin University

Although additive manufacturing (AM) offers exciting new opportunities for creating materials with different properties to their conventionally manufactured counterparts, there is still much to learn about the relationship between the properties and microstructural features of these AM materials in relation to their manufacturing parameters. In this paper, we will examine in detail these relationships for some steels, particularly AM SS316. Our focus has been on the AM manufacturing technique of laser powder bed fusion (LPBF) where a laser is repetitively scanned over a powder bed using a computer-generated pattern, thus manufacturing a part in a layer-by-layer fashion and generating some unique microstructural features. Some critical parameters for building parts in this fashion include laser power and speed, hatch width, scanning pattern, powder bed thickness and powder characteristics. In recent years we have used a variety of newer characterisation techniques, as well as some older ones, to extensively investigate the difference in the microstructure and corrosion resistance of AM SS316 prepared under a variety of processing conditions. For example, we have used X-ray CT in combination with SEM/EDS/EBSD and TEM/EDS to study porosity in the AM SS316, particularly lack-of-fusion pores, and have shown that this has been a major contributor to misinterpretation of some corrosion results published in the literature. We have also looked at the role of post-processing annealing treatments and found that it can significantly influence corrosion resistance, erosion corrosion resistance and passive film formation. The modification of passive film formation has led to more recent studies looking at passive film formation using Atom Probe Tomography.

Sciforum-060605: Polymeric smart coatings containing modified capped Halloysite nanotubes for corrosion protection of carbon steel

Sehrish Habib[1, 2], Adnan Khan[3], Salman M. Ismail[4], R. A. Shakoor[1], Ramazan Kahraman[5], Elsadig Mahdi Ahmed[2]

[1] Center for Advanced Materials (CAM), Qatar University, 2713 Doha, Qatar.
[2] Department of Mechanical and Industrial Engineering, Qatar University, 2713 Doha, Qatar
[3] Department of Materials Science and Engineering, Texas A&M University, College Station, 77843 TX, USA
[4] Community College of Qatar, Qatar
[5] Department of Chemical Engineering, Qatar University, 2713 Doha, Qatar.

A newly designed smart self-healing coating system comprised of modified halloysite nanotubes (HNTs) having end cap and the epoxy is proposed for corrosion protection of steels. In the first step, HNTs were loaded with 8-Hydroxyquinoline (8-HQ) used as a corrosion inhibitor. Then, the ends of the HNTs were sealed/capped using Cobalt (II) aiming for an efficient and controlled release of the loaded inhibitor. The smart coatings were developed by reinforcing loaded HNTs into the epoxy matrix and their structural, thermal, mechanical, and electrochemical properties were studied using various techniques. UV-Vis analysis depicted that the capping of the metal inhibitor complex was decomposed at acidic pH resulting in a controlled release of the loaded inhibitor into HNTs. Electrochemical impedance spectroscopic (EIS) analysis of blank and smart coatings demonstrated that the low-frequency impedance modulus of smart coatings reflected excellent corrosion inhibition performance as compared to blank epoxy coatings. The superior corrosion protection properties of smart coatings can be ascribed to the controlled and efficient release of the loaded inhibitor from the capped HNTs. This work confirmed the adeptness of 8HQ to mitigate the corrosion due to the controlled and effective release of the inhibitor from capped HNTs due to dissociation of the metal inhibitor complex (Co-8HQ).

Sciforum-060689: Electrochemical investigation and optimization of Olive leaves extract as a green anti-corrosion agent for Tin in acetic acid solution using response surface methodology

Sara Lahmady[1], Issam Forsal[1], Mohammed Ellaite[1], Khoula Dehhou[1], Khalid Benbouya[2]

[1] Laboratory of Engineering and Applied Technologies, School of Technology, Beni Mellal, Morocco.
[2] EMDD_CERNE2D, Mohamed V University in Rabat, School of Technology, 227 Crown Prince Avenue, Sal, Morocco.

Metal packaging, especially tin, is great for storing canned foods. The interaction of the food with the metal container reduces its shelf life due to the acidic nature of the canning solution, as corrosion can occur when the metals of the packaging dissolve. The inhibiting effects of olive leaves extracts on tin corrosion in 3% acetic acid were examined in this study. The impact of the concentration of inhibitor (0.1–1g/L), time (0.5–12h), and temperature (20–50°C) were investigated using a statistical method according to the design of experiment (DOE). For those three factors, response surface methodology (RSM) using Central Composite Design (CCD) was chosen and applied to the design matrix. A potentiodynamic polarization test was used to assess the input corrosion current density (Icorr) under various conditions specified in the design matrix. The model proved correct with a good coefficient of determination of (R^2 = 95.3%). The optimal processing parameters observed were: time: 2.86 h, temperature: 20°C and inhibitor concentration: 0.13g/L,
respectively. This study looked into the level of impact of every parameter on corrosion current density and included response surface plots and contour plots for each factor. According to the results, olive leaves extract molecules were adsorbed on the tin surface and developed a protective film layer that prevents the attack of water and CH3COOH(H+, CH3COO-) ions, reducing the corrosion process significantly. olive leaves extract is rich in organic compounds with heteroatom and π site in their molecular structures. When inhibitor molecules are introduced into an acidic solution, they get protonated, and these protonated molecules are physically adsorbed on the surface through electrostatic interaction with CH3COO-. The adsorption via the synergistic effect of the majority elements, as well as the minor components of the composition of the inhibitor used can be attributed to the inhibitory action of this extract.

Sciforum-060769: Evaluation of the effect of ciprofloxacin loaded into hybrid oxide-polymer coating on corrosion of Mg3Zn0.4Ca alloy

Lara Moreno[1], Cheng Wang[2], Sviatlana Lamaka[2], Mikhail Zheludkevich[2], Marta Mohedano[1], Raúl Arrabal[1], Juan Rodríguez-Hernández[3], Endzhe Matykina[1]

[1] Universidad Complutense de Madrid
[2] Helmholtz-Zentrum Hereon
[3] Instituto de Ciencia y Tecnología de Polímeros (ICTP-CSIC)

The protective capacity of functionalized hybrid hierarchical coating loaded with an antibiotic on Mg3Zn0.4Ca is discussed in this work. The coating comprises a porous ceramic oxide layer enriched in bioactive elements (Ca, P, Si) formed by plasma electrolytic oxidation (PEO). The pores of the PEO coating were sealed by a thin polycaprolactone (PCL) layer using a dip-coating technique. A porous PCL layer loaded with ciprofloxacin (CIP) was formed on top of the PCL-sealed PEO coating using a breath figures technique. The morphology and topography of the system were examined by SEM and optical profilometry. The release of the drug was investigated using UV/VIS spectrometer after 10 days of immersion in inorganic α-MEM. The effect of the drug liberated from the coating system on corrosion of Mg3Zn0.4Ca was evaluated using EIS, local electrochemistry experiments during 24 h (local current density by SVET, local pH, and dissolved H_2 concentration), and H_{-2} evolution test during 12 days in physiological conditions under flowing CO_2. The degradation rate of the CIP-loaded system was slightly lower compared to the drug-free system. This is due to the CIP release during the first hour of immersion that caused slight increase of the local pH reducing the aggressiveness of the environment.

Sciforum-060825: Impact of corrosion inhibition performance of smart epoxy coatings modified with yttrium oxide nanoparticles loaded with imidazole

Muddasir Nawaz[1], Nazal Naeem[1], R. A. Shakoor[1], Ramazan Kahraman[2], M. F. Montemor[3]

[1] Center for Advanced Materials (CAM), Qatar University, 2713 Doha, Qatar.
[2] Department of Chemical Engineering, Qatar University, 2713 Doha, Qatar.
[3] Instituto Superior Técnico, Universidade de Lisboa, Av Rovisco Pais, 1049-001 Lisboa, Portugal

Polymeric organic coatings are being developed as a result for effective corrosion protection solutions for metallic parts. Polymeric nanocomposite coatings that have been incorporated with corrosion inhibitors improved surface protection. In this study, yttrium oxide nanoparticles were loaded with the corrosion inhibitor imidazole and employed as additives in the formulation of an epoxy coating that was applied to a steel substrate. Fourier transform infrared spectroscopy (FTIR) confirms the changes in bonds after loading of corrosion inhibitor. Thermogravimetric analysis (TGA) shows the loading capacity of Y_2O_3 with imidazole. UV-vis examination revealed the imidazole's pH-sensitive activity, which aids in self-release when needed. The coating enhanced with Y_2O_3/IMD provides greater corrosion protection than coatings containing only Y_2O_3, which was revealed by electrochemical impedance spectroscopy (EIS) study of the coated samples. The presence of an imidazole forms the protective film on the steel substrate, which is confirmed by XPS analysis, improved the corrosion resistance of the coated samples.

Sciforum-060925: Improving corrosion protection of magnesium alloy by incorporating corrosion inhibitors into primer

Aun Nawaz Khan[1], Bahram Vaghefinazari[1], Cheng Wang[1], Ulrich Jüptner[2], Mikhail L Zheludkevich[1, 3], Daniel Höche[1], Sviatlana V Lamaka[1]

[1] Helmholtz Zentrum Hereon, Germany
[2] JUBO Technologies GmbH, Germany
[3] Kiel University, Germany

This work focuses on the development of an inhibitor-containing primer for an extruded Mg(MnCe) alloy. Several environmentally friendly corrosion inhibitors were selected and an easy-to-use approach involving direct admixing of corrosion inhibitor in a commercial primer coating was introduced. The primer was then applied on a Mg substrate pre-treated with a conversion coating. Tested corrosion inhibitors include several organic and inorganic salts. The barrier and active components of corrosion protection were tested by using Electrochemical Impedance Spectroscopy (EIS) and Scanning Vibrating Electrode Technique (SVET). Adhesion of the primer coatings containing the inhibitor was checked using pull-off and cross-cut tests. The overall corrosion protection performance was validated by exposing the primer-coated samples to a NSST for over 1000 hours. The results indicated an enhanced corrosion resistance of the coated alloy when the inhibitors were added to the primer coating. The strongest corrosion protection effect was achieved when cerium salt of weak organic acid was introduced into the primer.

Sciforum-059536: Inhibition of metallic degradation in corrosive solutions: a case study of isatin compounds

Taiwo Wasiu Quadri[1], Chandrabhan Verma[2], Lukman Olawale Olasunkanmi[3, 4], Omolola Esther Fayemi[1], Eno Effiong Ebenso[5]

[1] Department of Chemistry, School of Chemical and Physical Sciences and Material Science Innovation & Modelling (MaSIM) Research Focus Area, Faculty of Natural and Agricultural Sciences, North-West University, Private Bag X2046, Mmabatho 2735, South Africa
[2] Interdisciplinary Research Centre for Advanced Materials, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia
[3] Department of Chemistry, Faculty of Science, Obafemi Awolowo University, Ile Ife 220005, Nigeria
[4] Department of Chemical Sciences, University of Johannesburg, P.O. Box 17011, Doornfontein Campus, 2028, Johannesburg, South Africa
[5] Institute for Nanotechnology and Water Sustainability, College of Science, Engineering and Technology, University of South Africa, Johannesburg 1710, South Africa

Metallic degradation in corrosive media is a phenomenon of research interest in academia and industry because of its negative economic and environmental consequences on society. The application of corrosion inhibitors has been established as one of the cheapest, easiest and most effective methods of combating corrosion processes in industrial metals. Several authors have explored organic compounds as potential inhibiting materials because they possess numerous heteroatoms (N, O, P, S), polar functional groups, multiple bonds and aromatic rings. This study spotlights the use of isatin compounds as effective and environmentally friendly organic inhibitors for metallic degradation in different corrosive solutions. The inhibitive effectiveness of isatin compounds in various tested media using several testing techniques such as gravimetric, electrochemical, surface analytical and computational modelling are considered. The nature of adsorption and the mode of inhibition mechanism on metallic surfaces are also discussed.

Sciforum-061530: Interaction of organic inhibitors with metal surfaces studied by spectroscopic methods

Philippe Marcus[1]

[1] PSL University, CNRS-Chimie ParisTech, Institut de Recherche de Chimie Paris, Research Group of Physical Chemistry of Surfaces, Paris, France

Understanding the interactions between organic molecules and metal surfaces is key to the development of new inhibitors. In this lecture, we will interrogate organic molecule–metal surface systems using spectroscopic methods, Time of Flight Secondary Ion Mass Spectrometry, and X-ray Photoelectron Spectroscopy, combined with electrochemical measurements and corrosion tests. The nature of the interactions of MBT, MBI, carboxylates, and phosphonates with aluminium and copper will be presented and discussed. The experimental results will be compared to the results from DFT calculations.

Sciforum-061657: Laying the experimental foundation for machine learning in corrosion inhibitor discovery

Can Özkan[1], Lisa Sahlmann[2], Feiler Christian[2], Mikhail Zheludkevich[2], Peyman Taheri[1], J.M.C. Mol[1]

[1] Department of Materials Science and Engineering, Delft University of Technology, Mekelweg 2, 2628 CD Delft, The Netherlands
[2] Institute of Surface Science, Helmholtz-Zentrum Hereon, Geesthacht, Germany

It often takes 20 or more years to move a material to the market; however, after decades of research, the discovery of a successful green successor to the chromate-based corrosion inhibitors still eludes us. One promising approach to discovering inhibitors is the use of machine learning (ML), which has already shown potential in accelerating the pace of scientific discovery and the deployment of advanced material solutions. The main challenge of utilizing ML for corrosion research is the lack of high-quality datasets. Corrosion datasets are typically noisy and not often shared in a systematic and machine-readable way. Electrochemical data are generated with different electrochemical techniques at different times of exposure with different sample preparation procedures. This complicates combining and comparing the results from separate studies into one cohesive picture. To resolve this problem, we have created an extensive electrochemical inhibitor library of 80 inhibitor candidates. The electrochemical behavior of AA2024-T3 substrates in the presence of 72 small organic and 8 inorganic molecules was captured using linear polarization resistance, electrochemical impedance spectroscopy and potentiodynamic polarization techniques at different timesteps to obtain the most comprehensive electrochemical picture of the inhibition in the first 24 hours. The obtained experimental parameters can be employed directly as target parameters for training an ML model that is predictive of the performance of untested compounds to create a shortlist of promising candidates. Moreover, the experimental investigation yields additional input features that can be combined with molecular descriptors derived from the molecular structure and atomistic simulations. These input features exhibit great potential to develop augmented quantitative structure–activity relationships as they allow directly including information on the underlying mechanisms in the training of the models. The results of this study are expected to support the development of faster inhibitor screening techniques in the future, which can leverage the link between the molecular structure of the inhibitor and its corrosion activity.


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