Master Thesis subjects 2022-2023 proposed by

Research Group Electrochemical and Surface Engineering - VUB (SURF)

Topic 1: Understanding interfacial degradation of positive electrode materials in lithium metal batteries using a combined modelling-experimental approach

Summary:
Next-generation battery systems are playing a major role in the global shift towards a society based on renewable energy. Lithium metal batteries are leading this domain with a high power and energy density. However, challenges such as dendrite formation and solid-electrolyte interphase (SEI) formation due to the high reactivity of lithium metal highlight the need for a better understanding of interactions directly at the electrolyte-electrode interfaces. The goal of this project is to study the degradational behaviour of a electrolyte on a wide variety of positive electrode materials such as LMNO, LMO, NMC, LCO and variations in their surface facets. The researcher will be gain experience in computational chemical modelling using ab-initio molecular dynamics and density functional theory methods and will verify with experiments using surface analysis techniques (SEM, XPS, Raman,...) to identify decomposition products. This project offers a unique opportunity to collaborate in interdisciplinary research between chemistry and material science in this state-of-the-art research area.

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Topic 2: Surface properties and electrochemical performance of 3D-printed stainless steel

Summary:
Metal additive manufacturing (MAM), a process by which complex multifunctional metal parts are produced in a layer-by-layer fashion, is considered one of the enabling technologies for Industry 4.0. This technology has attracted a great deal of attention in recent years and has found numerous applications in industries such as medical implants, energy, aerospace, and automotive due to the fact that it allows near net-shape manufacturing of geometrically complex parts such as lattice structures and 3D structures with undercuts or cavities. Besides these industries, some MAM techniques (for instance direct energy deposition – DED – techniques) have also shown great potential for repair applications.
In contrast to conventionally manufactured alloys, the localized and rapid solidification achieved during MAM promotes the formation of a very fine microstructure with unique directional growth features. This special microstructure has been shown to play an important role in the mechanical performance as well as in the corrosion behaviour of these specimens. Although several studies have already been conducted in this area, there is still a lot to do to better understand the synergy between microstructure, post-thermal/surface treatments, and the mechanical/corrosion performance of these materials. This master project intends to do that. Through an extensive characterization of the additively manufactured specimens, the relation between microstructural features and defects with the functional/electrochemical surface properties will be established. The project will combine high resolution surface analysis (FE-SEM, EDX, XPS, UPS) with electrochemical testing (EIS, OCP-LSV, potentiostatic measurements).

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Topic 3: Operando study on the formation of conversion coatings

Summary:
Steel and aluminium alloys are used in many applications, including construction, transportation, consumer goods, etc. These materials require protection to prevent environmental degradation. In order to achieve this protection, organic coatings are often used. To increase the adhesion of these organic coatings, as well as improving the corrosion resistance, a conversion coating is often applied on their surface. Odd Random Phase Electrochemical Impedance Spectroscopy (ORP-EIS) is a technique that is able to characterize the different processes occurring in electrochemical systems, by looking at the impedance response as a function of the frequency. Recent advances in this technique allow for the calculation of the time-resolved impedance – unravelling the way the impedance changes in a small time window. The goal of this project is to investigate the formation process of conversion coatings operando, where the impedance is measured while the conversion coating is being formed. This will lead to new insights on the formation mechanism, and this information can then be combined with the performance of the conversion coating to understand how to improve the process. Aside from the electrochemical characterisation, the formed conversion coatings will also be analysed by Scanning Electron Microscopy (SEM) combined with Energy-Dispersive X-ray Spectroscopy (EDX) and X-ray Photoelectron Spectroscopy (XPS) to provide additional insights into the formation process and final corrosion barrier properties of the formed layer.

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Topic 4: Expedited ORP-EIS evaluation of the effect of Cu(II) at the interface of epoxy coatings with converted galvanized steel

Summary:
The corrosion protection of hot dip galvanized (HDG) steel is of great importance in the automotive industry. To this purpose, Zr-based conversion of the metal substrate (for passivation and improved adhesion), in combination with the application of a polymeric primer coating (which acts as a physical barrier to the environmental moisture and oxygen) is performed. Typically, Cu(II) additive is used as an accelerator in the Zr-based conversion. In this work, we want to investigate the effect of copper on the failure of the barrier properties of an epoxy-amine coating on the converted HDG steel substrate by odd random phase multisine electrochemical impedance spectroscopy (ORP-EIS), a singular method developed in our laboratory. High temperature and application of cathodic polarization will be applied in order to accelerate the breakdown of the polymer coating.

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Topic 5: Understanding the performance of novel catalytic materials for integrated photo- and electrochemical CO2 conversion processes: mechanistic insights by nanoscaled molecular surface characterization

Summary:
Design of complex photo-electrocatalyst material systems for CO2 conversion into methanol requires knowledge of the basic properties of each component's band structure in order to achieve efficient charge transport thus maximizing catalyst activity and selectivity towards methanol.
As the top surface of the catalyst is key in the efficiency of the conversion processes, X-ray Photo-electron Spectroscopy (XPS) in combination with Ultraviolet Photo-electron Spectroscopy (UPS) will be employed. XPS allows to identify with a 10 µm lateral resolution, the chemical configuration present at the first few nm's of the electrode material. UPS is even more surface sensitive and provides a complete characterization of the valence bands as well as useful electronic parameters of the catalysts such as work function, ionization energy and fermi level position. Knowledge of these parameters provides a level reference relative to the vacuum energy, which is important for applications where the discontinuities of energy levels between different materials have a large effect on the materials properties and performance.

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Topic 6: Finite element modelling of corrosion protection using inhibitor particles in an organic coating

Summary:
Metal corrosion has been a main factor in the high maintenance cost and the reduced lifetime of many structural projects. This has motivated many research efforts towards corrosion protection. Organic coatings are commonly used for that purpose. However, a coating defect would create a vulnerable location for severe pitting corrosion causing considerable damage to the metal. A favorable solution is the usage of inhibitor particles dispersed in the coating. In the case of metal surface exposure, the particles would diffuse to the defect to provide additional protection from the environment and prevent oxygen from reaching the surface.
The aim of the project is to model the protection provided by an organic coating with dispersed inhibitor particles in a scribe exposing the metal surface to the environment. Different inhibitors and modes of inhibition are considered. The model will take into account the reactions occurring at the surface for metal corrosion and inhibitor protection, as well as the transport of ions and the inhibitor particles through the coating and the exposed surface. This would be done using a finite element software tool. Some experiments could be conducted to obtain some of the model inputs or to verify the results.

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Topic 7: Designing of composite solid-state electrolyte for high performance all-solid-state lithium-ion batteries

Summary:
With rising gas prices due to war and the incredibly pressing need to rapidly transition away from fossil fuels, energy conversion and storage devices are getting a lot of attention. Over the last two decades, it has been confirmed that energy storage devices, more specifically, Lithium-ion batteries (LIBs), are a key enabling technology for many needs of our everyday life; for example, they have enabled the revolution of internet of things (how we share and communicate), and meanwhile inspired the development of full electrical cars. However, its applicability is currently limited by its use of liquid organic electrolytes, which are extremely flammable and hazardous, which pose a very serious safety risk and short lifetimes. As a result, in recent years there has been a considerable push toward the development of all-solid-state batteries and, specifically, new solid and/or semi-solid electrolyte materials. This project aims to design a new composite electrolyte (e.g., Polymer-Ionic-liquid electrolyte) with high lithium-ion conductivity and electro-chemo-mechanical stability for all-solid-state batteries. In this regard, understanding the role of different functional groups in the composite electrolyte is the key if the performance, lifetime and the safety of the electrolyte is to be improved. In this project, a hybrid multiscale computational approach alongside with experimental methods will be used to get new insights into mechanisms of lithium mobility with such a composite electrolyte.

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Topic 8: Investigation of Lithium-ion Batteries on Nanoscale

Summary:
In recent years, atomic force microscopy (AFM) have gained a lot of attention for investigating battery systems with a high spatial resolution (<50 nm). In this project, we will conduct a research on lithium-ion batteries with our state-of-the-art AFM facilities.
Kelvin probe force microscope (KPFM) is one of the extended AFM-based techniques. It enables mapping the surface potential on a variety of solid-state materials by measuring their characteristic work function. KPFM can be used to address the physical interfacial properties of battery systems with a high spatial resolution. Another essential technique is current-sensing AFM (CS-AFM), which can determine the local electrical conductivity of composite surfaces.
Apart from the surface characterizations, this project will also focus on advanced AFM studies on the cross-sectional surface of battery materials. The cross-section is prepared by an advanced ion-beam polishing method resulting in an ultra-smoothed surface, which allows AFM-based techniques to reach a nanoscale resolution on multiple important interfaces of Li-ion battery. This approach can be further extended to advance in-situ/operando analysis on solid-state lithium-ion battery systems. It will help to achieve dynamic insights with high spatial resolution on the buried solid-solid interfaces, which are often not accessible with conventional approaches.

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Topic 9: Effect of trace elements on the properties of 6060 aluminium

Summary:
Aluminium is a metal which can be very easily recycled without major changes in its properties. On top, the CO_2 emissions of aluminium production can be drastically reduced by using scrap material instead of bauxite as aluminium resource. However, the trace element content can increase beyond classical levels when using end-of-life material. Typical examples but not exclusively are iron, copper, zinc and manganese. The effects those increased levels of trace elements have on the final extrusion product are not yet fully understood. Specifically the effects the trace elements have during extrusion, heat treatment and pre-treatment processes like etching and anodizing require a better understanding to be able to maximize the recycle metal content in future 'greener' alloys.

Within this master thesis project the focus can be mainly put on one of the following points:

1. Maximizing the extrusion speed is very important for a companies. However, the highest possible extrusion speed depends on the alloying elements and the microstructure of the alloy during extrusion. In co-operation with the company EMAX extrusion parameters (e.g. billet temperature and ram speed) will be varied and the produced profiles will be analysed to determine the different influencing factors.
2. The heat-treatment process is primarily performed to increase the mechanical strength of an alloy. However, some researchers have shown that it can also have a big impact on the etching mechanism and thus on the visual appearance. What is not yet fully understood and requires further investigation is whether different trace element concentrations require different heat treatment procedures.
3. Extrusion profiles made from 6xxx aluminium alloys are typically chemically etched before the final protection layer of anodic aluminium oxide is applied. Two main etching mechanisms exist which depend on the composition of the alloy and the etching bath: preferential grain etching (PGE) and grain boundary etching (PGE). In acid, 6xxx Al usually etches along the grain boundaries. In alkaline solution both mechanisms can occur. When increased Zn levels are present, preferential grain etching (PGE) takes place which leads to an undesired spangling appearance of the aluminium profiles. Although, this fact is well known, the change in chemical etching mechanism is not yet understood.
4. Finally, trace elements influence the electrochemical formation of the anodic oxidation layer during anodizing. We would like to get a better picture of how the trace elements influence that formation and properties like layer thickness, colour and corrosion protectiveness. Furthermore, possible ways to adapt the alloys or the alloy processing to counteract negative effects should be developed.

For this master thesis the student can freely choose between the various surface analytical techniques, electrochemical techniques and mechanical methods available at the SURF group. Depending on the chosen topic, the student will work possibly closely in cooperation with the extrusion company for adaptation of the profile and sample processing.

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