1. Subject 1
Title: Surface properties of 3D printed metal: stainless steel by LMD
Title: Surface properties of 3D printed metal: steel by WAAM (in collaboration with the company OCAS/Arcelor Mittal and Guaranteed)
Summary:
3D printing or additive manufacturing (AM) offers the possibility to produce intricate shaped objects in one printing operation, whereas conventional processing implies that intricate shapes need to be produced by machining or welding of the different elements to obtain the final assembly. Furthermore, AM is also being considered for repair processes where worn or broken parts of a metallic product are repaired by AM, extending the product’s lifetime and conserving materials. The 3D printing by LMD and SLM start from metallic powder and for WAAM the starting material is metal wire, which is by the printing operation locally sintered to form the 3D shape. There is little insight in the surface properties of such 3D printed metals, for example towards the corrosion behaviour and surface treatments, such as anodising or chemical conversion.
In these master projects the challenge is to fully characterise the surface of 3D printed metal and relate it to the functional surface properties. Depending on the application various surface properties and tests need to be considered. These projects combine high resolution surface analysis with experimental testing (electrochemical analysis, surface treatments and corrosion testing).
We can accept two students on these topics.
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2. Subject 2
Title: Functional surface properties of recycled aluminium
Summary:
Recycling of aluminium results in alloys with higher levels of alloying elements. This generally does not affect the mechanical behavior of the alloys, but certain functional properties may change. In this project there is close collaboration with E-MAX, market leader in recycled extrusion profiles. The research deals with how recycling affects the surface behavior of the alloys. This project combines high resolution surface analysis with experimental testing (etching, anodizing, electrochemical conversion and corrosion analysis) of the recycled alloys.
We can accept two students on these topics.
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3. Subject 3
Title: Unravelling the role of Zr in the Si/Zr conversion coating on MaX1.2HY, a newly developed group of stainless steel
Summary:
Regarding the new environmental regulations in terms of greenhouse gas and fine particle emission, the automotive industry is looking for new high-strength materials in order to reduce part thicknesses and total weight. MaX1.2HY is a type of press hardening stainless steel that is dedicated to automotive structural parts and chassis parts. The automotive industry takes advantage of a multi-layer coating in order to have optimal
properties of the final product, one of these layers is conversion coating. Si/Zr combined conversion system is one of the novel choices for automotive applications. This research focuses on understanding how Zr in this conversion system improves the deposition of Si/Zr coating on this class of stainless steels.

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4. Subject 4
Title: Corrosion protective properties of conversion treatments on HDG steel in the presence of Cu additives
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, firstly, we want to investigate the corrosion properties of the converted substrate with and without presence of copper by odd random phase multisine electrochemical impedance spectroscopy (ORP-EIS), a method developed in our laboratory. This will be followed by the study of the influence of the Zr-based conversion with(out) Cu additive present at the interface between the HDG steel substrate and an organic coating on the barrier properties of the latter. In the end, the conditions for a better corrosion protection of the galvanized steel will be individuated.

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5. Subject 5
Title: Looking at the hybrid interface in metal-organosilane systems by a state-of-the-art surface analytical toolbox
Summary: Organosilane coatings are applied to metal substrates for corrosion protection and promotion of adhesion to polymeric primer coatings. The metal oxide – organosilane interface is crucial to the adhesion performance of the entire coating system. Nevertheless, interfacial molecular information, required to point out which chemical binding interactions are accountable for strong adhesion, is not easily obtained. In this project, state-of-the-art time-of-flight secondary ion mass spectrometry (ToF-SIMS) and X-ray photoelectron spectroscopy (XPS) techniques will be employed to study the metal oxide – organosilane interface. Argon cluster ions can be used to sputter thick coatings in order to make the buried interface accessible for a molecular analysis. Our new XPS instrument is also equipped with UV-photoelectron spectroscopy (UPS) to probe photoelectrons emitted from the valence band region. Important industrial process parameters such as curing temperature will have to be evaluated with respect to adhesion performance. A heating stage allows to study curing temperature in-situ with XPS/UPS.

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6. Subject 6
Title: Polymer/electrolyte interactions in high-performance organic coatings
Summary: One of the main applications of high-performance coatings is to protect the metal surfaces and acting as a barrier restricting the contact between metal and corrosive environments. Improving the protection performance of organic coatings require specific knowledge in failure mechanisms to ensure the maximum possible lifespan. The presence of water and ions can significantly influence the service life of the coating, causing degradation and failure of the coated metal system. In this research, an appropriate methodology will be designed to study the transfer of ions in the coatings using change in ionic conductivity in a concentration cell while their effect on interfacial bonds will be studied by FTIR in Kretschmann geometry integrated with ORP-EIS.

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7. Subject 7
Title: Machine Learning applied to the study of localised corrosion (in collaboration with the VUB Artificial Intelligence lab)
Summary:
Humankind has developed a metals-based civilisation by taking advantage of the stable surface properties of certain metals/alloys. The reason for this stability has been attributed to the existence of a thin reaction product on their surfaces: the passive film. However, in certain media, passive surfaces are susceptible to various forms of localised corrosion, leading to an extremely dangerous situation. The construction of an ML model is an inductive and interactive process, resulting in the discovery of unseen patterns. It relies upon a two-stage process: a subset of the data is used to construct and train the model, and subsequently, in a testing phase, unseen data is used for validation. This project will take advantage of the extensive scientific literature available at VUB databases. Several published articles dealing with passive metals exposed to variable experimental configurations will be selected, and meaningful electrochemical information will be imported to Python environment. Selected features displaying positive correlations with the data targets will be used to test ML algorithms. This question will be answered: which parameters influence localised corrosion the most?
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8. Subject 8
Title: Study of the copper electrorefining process and how to improve it
Summary:
Electrical apparatus/processes will only become more important in the future. The electrification of things, a concept describing the shift from fossil fuels towards (green) electricity to power everything, lies at the origin of the increasing demand. Battery or fuel cell powered cars, heating pumps and maybe even CO₂ conversion rely or might rely on electricity. High purity copper (99.995%) is an essential material to enable the electrification of things. This importance arises from the optimal conductivity versus cost ratio which characterizes copper.
The essential production step to produce high purity copper is electrorefining (ER). This process converts an impure copper anode into a pure copper cathode with the aid of electrical current and electrolyte (electrolysis). Unfortunately, this final step is challenged by a changing feed material, caused by increased recycling, and a demand to increase the current density, needed to decrease the processing time.
In this master thesis, you will investigate the electrorefining process of copper with a focus on the copper deposition to identify problematic process conditions. Electrochemical Impedance Spectroscopy will be used to study the plating process operando (performing an experiment while the process is running). Several other techniques (microscopy, SEM, AFM, XPS...) will be applied to investigate the finished product, the copper cathode.
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9. Subject 9
Title: What happens in lithium-ion batteries at the nanoscale during cycling?
Summary:
All-solid-state Li-ion batteries are considered as the revolutionary technology for the next-generation batteries. In recent years, atomic force microscopy (AFM) has gained a lot of attention for investigating battery systems with a high spatial resolution (<50 nm). In this project, we will conduct 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 characterization, 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 a Li-ion battery. This approach can be further extended to...
advance in-situ/operando analysis on solid-state Li-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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10. Subject 10
Title: Prediction of diffusion induced stress in lithium-ion battery materials through finite element modelling
Summary:
One of the critical challenges in advancing Li-ion battery technologies is fracture and decrepitation of the electrodes as a result of Li-ion diffusion during charging and discharging operations. When Li-ion is inserted in either the positive or negative electrode, there is a volume change associated with insertion or de-insertion. Diffusion-induced stresses can therefore cause the nucleation and growth of cracks, leading to mechanical degradation of the batteries. The goal of this master thesis is to use experimental data of thin film cobalt-free Li-ion battery electrodes and use this input in a Finite Element Model to predict the formation of mechanical stress in the electrode particles when cycling the battery. The model is made in Comsol Multiphysics starting from a given elementary model, and the experimental work includes surface analysis techniques (SEM), cell preparation in a glovebox and electrochemical characterization experiments (Cyclic Voltammetry, Galvanostatic Cycling).

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11. Subject 11
Title: Designing of composite solid-state electrolyte for high performance all-solid-state lithium-ion batteries
Summary:
Over the last two decades, it has been confirmed that energy storage devices, more specifically, Li-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 and 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 Li-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 Li-ion mobility with such a composite electrolyte.

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12. Subject 12
Title: 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. Li 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 Li 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 an electrolyte on a wide variety of positive electrode materials such as LMNO, LMO, NMC, LCO and variations in their surface facets. The researcher will 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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13. Subject 13
Title: Study of the influence of different conductive polymers as solid electrolytes on the performance of electrolytic capacitors

Summary:
Capacitors are, same as batteries, energy storage devices. Among the different types of capacitors, the so-called supercapacitors present high power density properties and rather high energy density values compared to their classic counterparts. While these will not substitute batteries, it is more common to find them as part of storage systems in hybrid or electric vehicles. Conductive polymers act as the solid electrolyte and they are not only good electrical conductors but also allow good contact between two porous electrodes. At the same time, conductive polymers allow larger temperature windows and avoid leakage risks. These materials are being recently rediscovered thanks to modelling experiments, but there are not many experimental studies yet. The goal of the project is to study the interaction upon different coating conditions between conductive polymers and aluminium electrodes. The project will cover from the sample preparation to the collection and interpretation of the electrochemical and surface analysis data (Electrochemical Impedance Spectroscopy and Atomic Force Microscopy).

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