Master Thesis subjects 2014-2015 proposed by
SURF – Research Group Electrochemical and Surface Engineering

Each of the subjects are promoted by one of the following professors: Iris De Graeve, Annick Hubin, Herman Terryn, Yves Van Ingelgem, Isabelle Vandendael. For more information on the subjects, please look at the SURF website: http://www.surfgroup.be/education

1. Investigating the working principle of self-healing coatings using the properties of high-resolution local EIS measurements

**Summary:** Local Electrochemical Impedance Spectroscopy (LEIS) is an emerging discipline in the field of electrochemical research. It is based on the widely accepted Electrochemical Impedance Spectroscopy (EIS) technique, a powerful method to determine reaction mechanisms on macroscopic electrodes. When however the electrode represents a heterogeneous behavior, local information is indispensable. This project consists of further integrating the concept of localized EIS measurements and atomic force microscopy (AFM). As such a setup will be further developed that generates high-resolution topographical information as well as local EIS spectra.

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2. Development of a high throughput drug discovery tool

**Summary:** Electrical impedance spectroscopy permits the label-free detection of the activation of mammalian cells. In practice, however, the activation cannot always be detected. Moreover, commercial instruments use only one or a few measurement frequencies, potentially losing valuable information. The signal also gives only limited insight into the cell properties that were altered by the stimulus. The aim of the project is to improve the dielectric spectroscopy measurements by greatly extending the frequency range over which the electrical properties of the cell monolayer are measured. The ultimate goal is to include complementary biological measurements to discover the electrochemical fingerprint of known biochemical reactions.

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3. Development of new concepts for State of Health monitoring of batteries and battery stacks

**Summary:** As certain reliability is desired from battery-powered vehicles, it is essential to be able to assess the state of health of such a battery at regular time intervals. Optimally this would happen without temporary loss of functionality for the user. This is where impedance spectroscopy (IS) steps in. IS is a tool widely used in electrochemistry, for example in the design of new battery cell concepts. It is based on applying a low amplitude AC stimulus to a system and subsequently recording its response. Dividing stimulus and response allows determining the transfer function of the system under test. The thesis work will consist of testing a number of batteries in various conditions. Subsequently a model is constructed for this system, including temperature, state of charge and other relevant parameters.

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4. Hybrid interfaces: reaching the interface between polymers and metal oxides

**Summary:** Coatings are widely used to protect materials from corrosion, enhance their durability, optimize their functional properties, ... Most of the time, the combination of polymers deposited on metal oxides is used. However, although these coatings are widely used, it is not known how these films are formed on the
As in tradition polymer coatings it is very difficult the buried interface, this project focuses on the development of nanometer thin polymer films. These structures will be deposited on optimized metal oxides, where top surface sensitive (vacuum) techniques will be used to gather information about the interface. The aim of this work is to bring a deep understanding to the molecular bonding and adhesion strength at the polymer/(hydr)oxide/metal interfaces.

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5. The use of local potential and electrochemical techniques to study the hydrogen embrittlement of steel

Summary: High strength steels are good candidates for many structural applications. However, when these materials come into contact with a hydrogen containing environment, hydrogen changes the properties frequently leading to failure. This problem is called hydrogen embrittlement (HE). The HE phenomenon is still fully not understood.

This project is in collaboration with UGent for the microstructure and texture characterization. At VUB the local electrochemical study will start up. This is a new topic in the SURF group with exciting challenges, exploring the use of the local potential and electrochemical techniques (e.g. SKFPM) to locate H in the complex steel microstructure and determine its effect in the material on a small length scale.

Contact: Iris De Graeve - idgraeve@vub.ac.be

6. Mechanism of Ni electrodeposition from electrolytes containing amino acids

Summary: Despite its long history, electrodeposition of metallic coatings is still one of the widely used industrial techniques to improve properties of initial substrate. As non-toxic and easily recyclable complexing agents, amino acids are very promising for nickel electroplating. However, in order to control the deposition process and predict properties of the coating clear understanding of the process mechanism is required.

The project includes both experimental and modeling parts. The process kinetics and coatings quality will be measured and a possible mechanism of the process will be proposed based on these data. Then, numerical model will be build using dedicated in-house software in order to confirm suggested mechanism and make some predictions about optimal conditions of nickel electrodeposition.

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7. Electrocatalyst screening for a cogeneration fuel cell

Summary: Cogeneration fuel cells are fuel cells that are used to produce chemicals with electricity as a by-product. An example is the production of hydrogen peroxide form oxygen and hydrogen. By letting hydrogen and oxygen react to hydrogen peroxide instead of water, less electricity is generated, but a valuable chemical compound is obtained.

This master project aims at finding a suitable catalyst to produce hydroxylamine from nitric oxide in a fuel cell. Hydroxylamine is an important material for the production of nylon. The project will consist mainly of electrochemical measurements, but will also involve characterisation of the catalyst materials.

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8. Development of a new Co free coating for steel cord in tires

Summary: Adhesion performance of steel cord with the rubber compounds of the tire is one of its most important product properties and an inherent safety feature. To obtain a good adhesion performance, all tire manufacturers add cobalt fatty acids to their rubber compound formulations. Recently, some cobalt species have been defined as Substances of Very High Concern. Hence, there is an urgent need to come up with a new and maybe even better performing coating and adhesion system, as most tire makers are striving
to increase the sustainability of their products. In addition, cobalt-free compounds are also expected to age slower and to have longer fatigue life.

In this Master thesis we want to study (metallic) coatings and their related technologies, applicable for steel cord, that have the potential to generate equal to better adhesion performance, and allow cobalt adhesion promoters to be completely removed from the rubber compounds. The master thesis will be in collaboration with Bekaert Company.

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9. Electrodeposition of electroactive nanostructures from ionic liquids

Summary: Supported nanostructures are important for a variety of practical applications, specially electrocatalysis and energy conversion devices. In contrast to other synthesis methods, electrochemical deposition allows the growth of the nanoparticles directly on the final support, obtaining enhanced properties. Recent work carried out in the research group has shown that under certain conditions, nanostructures grow by aggregation of very small nanoclusters (d ≈ 1-3 nm). In this thesis, you will evaluate ionic liquids as electrolytes for the electrodeposition of different nanostructured materials. The ultimate goal is to control electrolyte-nanocluster interactions to obtain nanostructures with enhanced electrochemical properties. You will use different electrochemical apparatus and state of the art characterization techniques such as FE-SEM, FE-Auger, XPS or AFM.

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10. Measuring of the electrical conductivity of mixed ionic/electronic conductors through EIS

Summary: Yttrium doped ceria (Y$_{x}$Ce$_{1-x}$O$_{2-x/2}$) is a ceramic material which is a mixed ionic electronic conductor. It has important applications in oxygen sensors, as catalyst material and as electrolyte or cathode in solid oxide fuel cells. The electrical conductivity of this material is strongly dependent on microstructure, temperature and oxygen partial pressure, both in magnitude and in type (ionic/n-type/p-type semiconductor). At SURF we currently examine thin nanocrystalline films of this material, which have unique properties when compared to bulk materials.

As a student working on this project, you perform electrochemical impedance spectroscopy (EIS) measurements on these films, you analyze the results and you compare the obtained conductivities to literature data and simulation results. Furthermore you collaborate in developing a technique to distinguish between ionic and electronic conductivity in the measurement results. As such your work will expand the knowledge on mixed conductors and improve powerful and innovating measurement techniques.

Contact: Dries Van Laethem – dvlaethe@vub.ac.be

11. Modeling of the electrical conductivity of mixed ionic/electronic conductors

Yttrium doped ceria (Y$_{x}$Ce$_{1-x}$O$_{2-x/2}$) is a ceramic material which is a mixed ionic electronic conductor. It has important applications in oxygen sensors, as catalyst material and as electrolyte or cathode in solid oxide fuel cells. The electrical conductivity of this material is strongly dependent on microstructure, temperature and oxygen partial pressure, both in magnitude and in type (ionic/n-type/p-type semiconductor). At SURF we currently examine thin nanocrystalline films of this material, which have unique properties when compared to bulk materials.

As a student working on this project, you perform finite element simulations of a thin film – electrode assembly. You evaluate different models for charge carrier transport and electrode junctions. Finally you compare your simulation output to measurement data to identify material parameters. As such your work will expand the knowledge on mixed conductors and improve powerful and innovating simulation techniques.

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12. Determining a reliable algorithm for the factor analysis of Auger Electron Spectroscopy (AES) data

**Summary:** Auger Electron Spectroscopy (AES) is a very powerful surface analysis technique. It allows the study of material’s surfaces (upper 5 to 75 Å) with a lateral resolution going down to 10 nm. Besides the elemental chemical information, chemical compounds can be identified from recorded Auger data using some mathematical tools, like factor analysis (FA). During a FA, first the number of principal components needed to rebuild the experimental data set is determined. In a second step, these principal components can be identified using some standards of the chemical compounds suspected to be present in the sample under study. In this thesis, a new approach for determining the number of relevant principle components will be developed that takes into account the measurement uncertainty. The proposed method requires at least 2 independent measurements and some advanced data processing techniques developed at the department ELEC. The data processing will be performed in Matlab®. As a continuation of previous research, we will use nitrided iron samples as standard samples to establish the reliable algorithm for the factor analysis.

**Contact:** Isabelle Vandendael – ivddael@vub.ac.be


**Summary:** In many applications the used materials, especially metals, are protected from the environment by applying a coating. In this context the use of Self-healing coatings has become an interesting research topic. These polymeric coatings have the property of self-repair by either an intrinsic, for example by using a shape memory polymer, or an extrinsic mechanism, for example by incorporation of encapsulated healing agents. Additionally for corrosion protection of metals, corrosion inhibitors may be incorporated in the coating for multiple action healing. In the present project the focus is on the development of self-healing coatings for use in and on reinforced concrete. This is a new research topic, as part of a large scale project with several industrial applications, for example off-shore structures, bridges and tunnels, large buildings, where repair and maintenance must be reduced to a minimum.

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14. Effects of recycling on the functional properties of aluminium extrusion alloys

**Summary:** Recycling increases the levels of alloying elements and introduces unintentional elements into the alloys. This generally does not affect the mechanical properties of the alloys, but conversely certain functional properties may differ. For example, the optical appearance after anodizing and the filiform corrosion susceptibility after painting, two issues to be dealt with when considering recycled alloys for example for building applications.

In this project the effects of recycling on the microstructure and composition of 6000 series extrusion alloys will be linked to the appearance and corrosion properties. For this detailed material characterization using various surface analytical methods such as field-emission scanning electron microscopy combined with energy dispersive X-ray analysis (FE-SEM/EDX), Auger electron spectroscopy (AES) and X-ray photoelectron spectroscopy (XPS) will be performed for the bulk and surface characterization of the recycled alloys and compared to the primary alloy. The microstructural and compositional variations will then be related to the anodizing behavior, resulting appearance properties, and corrosion performance.

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15. Electrochemical behaviour of a shape-memory alloy for biomedical applications

**Summary:** Shape-memory alloys are in biomedical applications typically used for example for cardiovascular stents and orthodontic wires. The best known shape-memory alloys show a thermally triggered shape-memory behaviour, such as Nitinol - a titanium-nickel based alloy. A new generation of shape-memory alloys responds to a magnetic trigger, opening the path to other applications, for example, in advanced prosthetic devices.

For most applications, besides the mechanical properties also the corrosion behaviour of the metals
determines their potential use. For biomedical devices this is also a critical issue. In this project the electrochemical properties of a new type of shape-memory alloy will be investigated in relation to its microstructure.

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16. Study of the leaching-out process of inhibitors incorporated in organic coatings

Summary: This study is part of a project where different inhibitors for zinc and hot dip galvanized steel are compared on their ability to be incorporated into organic coatings. Secondly their leaching-out process will be monitored with advanced local electrochemical methods. Scanning Vibrating Electrode Technique (SVET) allows the measurement of the electric field in solution by means of a vibrating microelectrode. As a result potential or ionic current density mappings can be recorded. Scanning Ion-selective Electrode Technique (SIET) is a micro-potentiometric technique which allows the determination of the concentration of an electro-active species is determined; the redox reaction cycle between the ultra-microelectrode tip and the surface allows the discrimination of areas of different substrate activity. All these techniques enable one to follow the leaching-out process in-situ and with high spatial resolution delivering important information on the mechanism.

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17. The study of eco-additives for the creation of multifunctional properties in self-healing coatings

Summary: For this research topic a collaboration between the Research group Electrochemica Land Surface Engineering and the Biotechnology department of VUB will be setup to explore the possibilities of using enzymes as eco-additives for the creation of functional properties in coatings. In this project we will explore the potential use of enzymes to substantially improve the functional performance of self-healing coatings. Encapsulated enzymes will be considered as additives for the protection against, and healing of coating damages caused by, microorganisms, with minimized health and environmental impact. Additionally, their use as catalysts for autonomous self-healing of coatings will be explored, as an innovative approach to be considered for example for offshore applications where healing must be fully autonomous.

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18. The electrochemistry of zinc and zinc alloys: Studied by synergistic use of traditional and novel techniques

Summary: Corrosion is a complicated process, since it is influenced by different factors such as the environment, the electrolyte solution etc. At SURF numerical modeling is applied to the interactions that govern corrosion processes. Obviously, reliable input is required to produce representative simulations and to make relevant predictions. The model is a bridge between experimental studies and real life corrosion problems. This bridge can only be solid if the building blocks are put stable. The building blocks of the model are the kinetic and thermodynamic parameters of the ongoing processes. The focus of this thesis will be the study of zinc and zinc-alloys to systematically obtain these parameters. A synergistic use of multisine EIS (electrochemical impedance spectroscopy) and local electrochemical methods will yield a richer knowledge with much greater insights into the electrode-electrolyte interface. At the same time relevant information on the formation of corrosion products is obtained.

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