DTU Energy Conversion
Department of Energy Conversion and Storage

Master's Projects

at

DTU Energy Conversion

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Master projects - Department of Energy Conversion and Storage

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19	Protective coatings for the improvement of corrosion resistance of porous steels for Solid Oxide Fuel Cells	ceramic processing	microscopy, microstructural analysis	solid oxide cell
20	valuation of Nb-doped SrTiO3 SOFC anodes modified with other transition metals (W, Mo, Fe,Cr, Cu)	ceramic processing	microscopy, microstructural analysis	solid oxide cell
14	Fabrication of Solid Oxide Cell Stacks by Ink-jet Technology	computing	electrochemical characterization, microscopy	solid oxide cell
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3	Analysis of Lithium Battery Electrodes by Impedance Spectroscopy	electrochemical characterization		Li-ion battery
4	Nano-structured coatings for high performance metal-supported SOFC	electrochemical characterization	microscopy	solid oxide cell
5	Three-Electrode Investigations of Critical Interfaces and Processes in Li-ion and Li-Air Batteries	electrochemical characterization	microscopy	Li-air battery
11	Degradation/passivation of mixed ionic and electronic conducting oxygen electrodes	electrochemical characterization	microscopy, ceramic processing	solid oxide cell
16	Understanding and optimising the low temperature reduction of Ni/(Sc)YSZ SOFC anodes	electrochemical characterization	microscopy	solid oxide cell
17	Infiltrated Ni-(Sc)YSZ SOFC anodes for improved carbon and sulfur tolerance	electrochemical characterization	microstructural analysis	solid oxide cell

25	Test of components of a carbon-oxygen battery	electrochemical characterization	catalytic characterization	carbon-oxygen battery / solid oxide cell
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27	New electrocatalysts for effective water splitting in alkaline solutions	electrode/materials development	electrochemical characterization	alkaline cell
28	Construction and electrocatalytic activity for medium temperature energy systems.	electrode/materials development	electrochemical characterization	PEM cell
1	Microstructures of new fuel cell materials	microscopy		solid oxide cell
8	Two and three dimensional SOFC anode microstructure characterisation	microscopy		solid oxide cell
9	Improving SEM based X-ray micro tomography resolution	microscopy		various
10	New methods for the alignment of three dimensional electron backscatter diffraction image stacks	microscopy		various
18	In situ surface study with high temperature scanning probe microscopy	microscopy		solid oxide cell
24	High performance SOFC Anodes Based on Infiltration of Ni-Ce0.8Gd0.2O2	microscopy, microstructural analysis		solid oxide cell
22	Novel techniques of thermo-mechanical characterization for lifetime prediction in glass-ceramic sealings	thermomechanical analysis	microscopy, microstructural analysis	solid oxide cell
23	Novel Sealing Strategies for Metal Supported Solid Oxide Fuel Cells	thermomechanical analysis	microscopy, microstructural analysis	solid oxide cell

29	Organic synthesis of light harvesting materials for polymer solar cells	synthesis and characterization	Polymer solar cells

Project 1: Microstructures of new fuel cell materials

Solid oxide fuel cells for electrochemical conversion of gas to electricity consist of granular layers of various ceramic materials. In the new generations of fuel cells nanoparticles of an active catalyst material are also infiltrated into the structure. The structural and compositional evolution of the nanoparticles in the harsh environment of reactive gas and high temperature during fuel cell operation has significant impact on the degradation and life-time of the cell. Studying the interaction between the nanoscale electrocatalyst and the micrometerscale ceramic backbone is thus of crucial importance for understanding and improving the performance of the resulting fuel cell.

This project will focus on studying this interaction in relation to the on-going research projects in the Department. The project will be experimental, and the techniques to apply will be scanning electron microscopy and transmission electron microscopy studies of sections of the fuel cells after they have been exposed to various test conditions. The microstructural studies will be related to the fabrication processes and the electrochemical performance as performed by colleagues in the Department.

The learning objectives will be accommodated to the student's wishes and prerequisites.

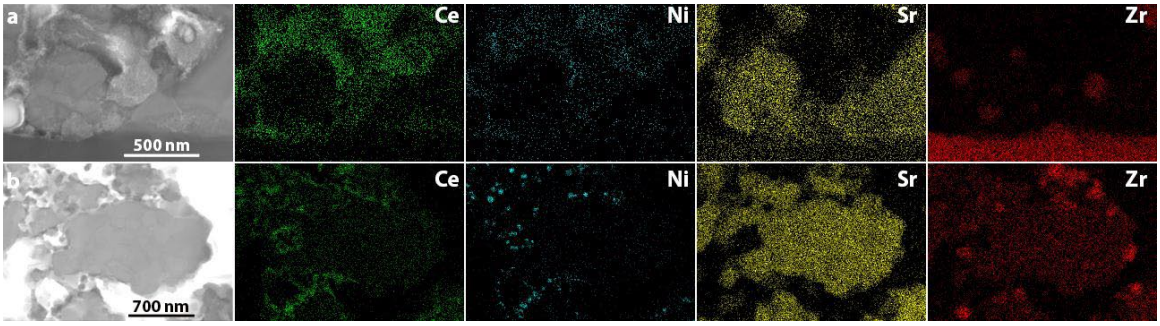


Figure 1: An example of elemental analysis of a fuel cell electrode by TEM before and after electrochemical operation showing the nanoscale changes of the materials.

Supervisors:
Luise Theil Kuhn, luku@dtu.dk, Wei Zhang, wzha@dtu.dk, and Peter Stanley Jørgensen, psjq@dtu.dk.

Project 2: Degradation of SOFC anodes – effect of anode performance on long-term stability

Recent results have shown that the degradation of Ni/stabilized-zirconia anodes is (besides many other factors) also linked to the initial anode performance i.e. the overpotential of the anode. This project aims to study the

interplay between the initial anode performance (i.e. resistance of the anode) at the starting point of long-term galvanostatic fuel cell testing and the subsequent degradation behaviour of the Ni/stabilized-zirconia SOFC anodes e.g. via poisoning cell test experiments.

Main Supervisor: Anne Hauch (Senior Researcher)
Co-Supervisors: Christopher Graves (Researcher)
Supporting project: Smart grid ready SOFC, FORSKEL

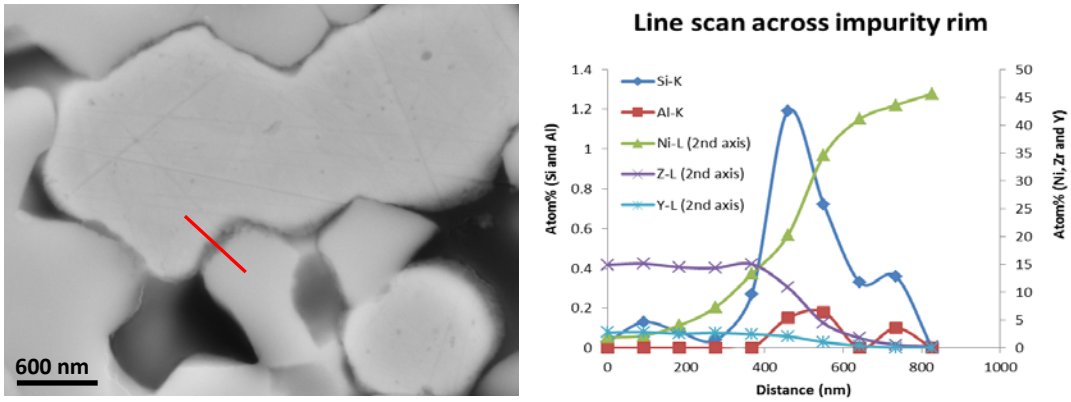


Figure 2: Silica containing impurity in the Ni/YSZ anode for degraded long-term tested SOFC.

Project 3: Analysis of Lithium Battery Electrodes by Impedance Spectroscopy

When batteries are used they heat up due to their internal resistance. This limits the efficiency and power and thus a low internal resistance is highly desirable. Both the two electrodes and the electrolyte of batteries contribute to the internal resistance but unfortunately it is often not very easy to find out how much each of the two electrodes contributes.

Impedance spectroscopy is one of the most frequently used techniques to investigate the electrochemical processes in batteries and the associated internal resistance. Unfortunately, the responses from the two battery electrodes very often overlap in the impedance spectra.

An interesting method to reveal the response from each electrode is to analyze batteries in a new type of measurement setup we name the H-setup. In the H-setup the liquid electrolytes of two batteries are connected. This makes it possible to change the state of charge (SOC) of one of the battery electrode at a time. The electrode impedance changes with SOC. By subtracting two impedance spectra measured with identical SOC at one electrode but different SOC at the other electrode it is possible to analyze the impedance of a single electrode of the battery.

The project aims to modify two commonly used lithium battery test setups know as a coffee-bag setup and the swage-lock setup to make two H-setups. The H-setups will be used for detailed impedance analysis of the lithium battery electrodes.

Swagelock cell

Coffee back cell

Supervisors

*Søren Højgaard Jensen,PhD,Senior Researcher, DTU Energy Conversion, shjj@dtu.dk
Jonathan Højberg, PhD student, DTU Energy Conversion
Torben Jacobsen, PhD, Ass. Prof. Emeritus, DTU Chemistry

Project 4: Nano-structured coatings for high performance metal-supported SOFC

Supervisors:

Peter Blennow (Senior Scientist), email: pebl@dtu.dk, phone: 4677 5868
Bhaskar Sudireddy (Scientist), email: bhsu@dtu.dk, phone: 4677 5640

Short description

The use of nano-structured coatings, obtained via infiltration, has shown excellent results with respect to high electrochemical performance and significantly improved corrosion resistance of metal supported SOFCs. However, further improvements are still required. The dual effect of nano-structured coatings is a promising route and the synergistic effect should be further developed and implemented by investigating novel materials and combination of materials.

Background

The present design of metal supported cells, developed at DTU, has demonstrated potential for the use in Auxiliary Power Unit (APU) applications. However, there is a need for further improvements of the cell components for long term durability in stationary applications. The use of nano-structured coatings, obtained via infiltration, has shown excellent results with respect to high electrochemical performance and significantly improved corrosion resistance of the metallic components in the metal supported cell. In the present design a combination of Gd-doped CeO_2 (CGO) and Nickel is used, where the CGO is responsible for the improved corrosion resistance and Ni acts as the main electocatalyst in the hydrogen dissociation reaction. CGO furthermore provides additional oxygen ion conductivity in the anode layer. However, further improvements are still required. The dual effect of the nano-structured coatings is a promising route and the synergistic effect should be further developed and implemented by investigating novel materials and combination of materials.

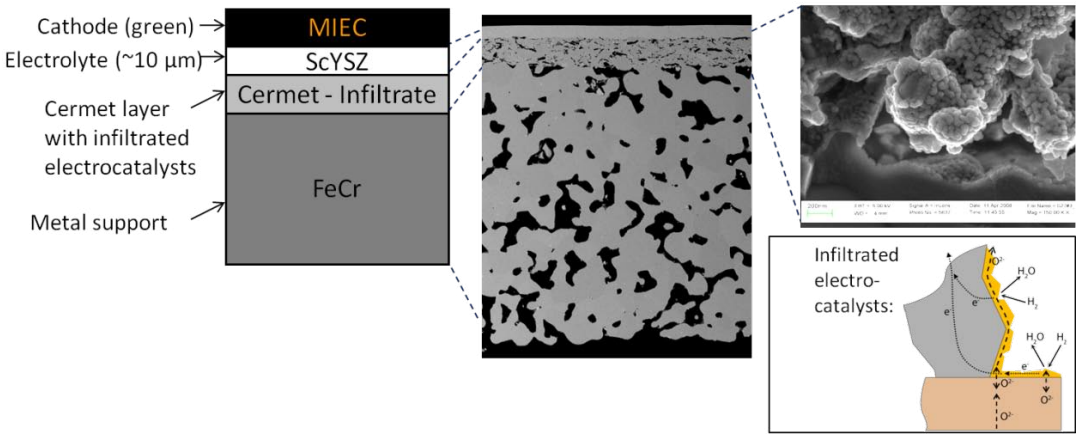


Figure 3. Schematic illustration together with a SEM image showing the concept of the metal supported cell design.

Project description

By modifying and/or controlling the properties of various surfaces/interfaces one can achieve better performance and durability. The project aims at improving the understanding of the infiltration technique of some selected nano-structured materials in order to improve critical surfaces/interfaces in the metal-supported SOFC design. Such a project could include, but not be limited to:

- Literature study to identify promising materials that could be used in combination with the stainless steel in the metal-supported SOFC.
- Develop an infiltration route to form a nano-structured coating on the metallic surfaces in the porous metal structure.
- Investigate the corrosion behavior of the coated stainless steel materials.
- Investigate the electrochemical behavior of the coated materials using electrochemical impedance spectroscopy to understand its effect as an electrocatalyst.
- XRD, SEM/EDS and or other relevant characterization techniques to investigate the morphology and composition of the nano-structured coatings.

Project 5: Three-Electrode Investigations of Critical Interfaces and Processes in Li-ion and Li-Air Batteries

Supervisors:

Johan Hjelm (main supervisor), johh@dtu.dk
Søren Højgaard Jensen (co-supervisor)
Jonathan Højberg (co-supervisor)

Project Description (5-line summary):
The Li-Air battery is a promising battery technology but is also associated with some significant challenges that must be overcome in order to realize its' potential. This project will investigate key processes and properties of components in Li-Air batteries by use of a three electrode set-up, which allows investigation of a single electrode of interest. Three-electrode investigations will also be carried out to characterize electrochemical Li-insertion (intercalation) reactions in state-of-the art Li-ion battery materials.

Detailed Project Description:
The Li-Air battery is presently receiving a large amount of attention due to the potential of this type of battery chemistry to realize significantly larger specific capacity than that possible with cells based on conventional Li-ion battery chemistries. Two of the key challenges with reversible Li-Air batteries are related to the poor conductivity of Li2O2 (lithium peroxide), and the formation of detrimental interfacial reaction products at the cathode ("air electrode"), which limits the reversibility, the capacity, and the efficiency of the cells at present. Transport and solubility of molecular oxygen in select organic aprotic solvents are also of importance for Li-Air cells.
Three-electrode set-ups are often used in electroanalytical chemistry and one of the main benefits is the possibility to investigate electrochemical processes taking place at a single electrode of interest. Another advantage is the precise control of the available free energy of reaction (via the cell potential) that is obtained in this configuration.
This project will be centered around three-electrode investigations of the properties of carbon electrodes (presently used as air-electrodes in Li-Air cells) with electrodeposited Li2O2 layers, and investigate strategies for enhancing the conductivity these layers. An increased conductivity of solid Li2O2 would improve the charge storage capacity of the Li-Air cell and is therefore of great interest. The conductivity of the Li2O2 layer will be probed by monitoring of the heterogeneous electron transfer rate of a well known outer-sphere redox couple. Three-electrode investigations will also be carried out to characterize electrochemical solid state Li-insertion (intercalation) reactions in state-of-the art Li-ion battery materials.

Main Methods:
Cyclic and Pulse Voltammetry, Chronoamperometry, Electrochemical Impedance Spectroscopy, Microelectrodes. Electron Microscopy and various surface characterization techniques may also be used depending on the outcome of the project.

Project 6: Electrode development for alkaline electrolysis cells operating at elevated pressure and temperature (50 bar, 250 °C)

Supervisor
Christodoulos Chatzichristodoulou, ccha@dtu.dk

Short description
We have recently demonstrated an advanced alkaline electrolysis cell concept capable of operation at temperatures up to 250 °C at 40 bar (thereby producing pressurized H2 and O2) with a current density of more than 1 A/cm^2 at nearly 100% efficiency. The aim of this project is to further develop the O2 evolving electrode in terms of performance and stability by implementation of Co-based electrocatalysts and leaching agents for microstructural optimization.

Renewable energy is an increasing part of our energy supply system, bringing forward the need for large scale energy storage. Hydrogen production through electrolysis of water is one promising method to achieve this. Alkaline electrolysis cells with metal foam based gas diffusion electrodes and concentrated aqueous potassium hydroxide as immobilized electrolyte in a meso-porous SrTiO3 structure have been developed and shown to operate at temperatures up to 250 °C at 40 bar [1, 2]. Current densities of 1.1 A/cm^2 and 2.3 A/cm^2 have been measured at a cell voltage of 1.5 V and 1.75 V, respectively, without using expensive noble metal catalysts. The high electrical efficiency and current density combined with relatively small production costs can lead to both reduced investment and operating costs for hydrogen and oxygen production. Preliminary "long-term" measurements have shown stable cell performance for 350 hours. Further optimization of electro-catalyst materials, electrode microstructure and cell reliability/stability needs to be carried out.
From electrochemical testing of cells with reference electrodes, it has been concluded that the oxygen evolution reaction (OER) is the most sluggish one. This project aims at exploring various electrocatalyst materials for the OER, such as Raney-Co, Co-based perovskites, and infiltrated metal foams and electronic conducting backbones. In order to separate the electrochemical contribution from the OER, circular OER electrodes of ca. 1mm diameter will be tested, using a much larger (ca. 10mm diameter) counter electrode for the hydrogen evolution reaction (HER). Half cells (ca. 10mm diameter button cells) of Ni foam and meso-porous SrTiO3 will be used (produced routinely) to screen print the OER catalyst. Cell testing will be carried out with EIS and CV in established autoclave test rigs.

Project 7: Novel nano-catalysts for NH_3 synthesis

Supervisor
Christodoulos Chatzichristodoulou, ccha@dtu.dk

Short description
A cleaner and more sustainable way to produce ammonia, as compared to the Haber-Bosch process used today, is one of the largest chemical challenges of our days, and forms the goal of this project. The idea is to combine N_2 and H_2O electrochemically into NH_3 (and O_2). An electrochemical cell will be constructed with a proton conducting electrolyte. Steam, fed at the anode of the cell, will be oxidized into H^+ and O_2. N_2, fed at the cathode of the cell, will be combined with H^+ and electrons to form NH_3.

Detailed description
Increased understanding and use of synthetic fertilizers played an important role in the industrial Green Revolution of the 20th century. It is estimated that almost half the people on Earth are currently fed as a result of the use of synthetic nitrogen fertilizer. Inorganic fertilizer is synthesized using the Haber-Bosch process, which produces ammonia as the end product, a feedstock for other nitrogen fertilizers. A 2002 report suggested that the production of ammonia consumes about 5% of the global natural gas production, which accounts for almost 2% of the world energy production.
Clearly, a cleaner and more sustainable way to produce ammonia is needed. This is in fact considered as one of the most important subjects in chemistry, and forms the goal of this project. The idea is to combine N2 and H2O electrochemically into NH3 (and O2). An electrochemical cell will be constructed with a proton conducting electrolyte and gas diffusion electrodes. Steam, fed at the anode of the cell, will be oxidized into H^+ and O2. N2, fed at the cathode of the cell, will be combined with H^+ and electrons to form NH3.

The main challenge of the project is to develop efficient electrocatalysts for the cathodic reaction. The rate limiting step is expected to be the dissociation of the N2 molecule. Recent DFT calculations have shown that this process can be significantly enhanced on surface vacancies of transition metal nitrides. Unfortunately, the formation of such vacancies is not favored energetically. In addition to that, the most promising metal nitrides are thermodynamically unstable under the required operating conditions. To overcome these limitations, we propose the use of well dispersed nano-particles of selected transition metals (Fe, Mo, W, Ru) onto surfaces of oxides and oxynitrides that posses a large number of surface vacancies, since such surface vacancies may also be expected to be favorable sites for N_2 dissociation.
Composite cermet backbones of $Ba(Ce,Zr,Y)O_3$ (BCZY) and $Sr_2(Fe,Mo)O_6$ will be screen printed on solid BCZY electrolytes. Fe,Mo nanoparticles are known to exsolve from Sr2(Fe,Mo)O6 upon reduction. Further infiltration with Fe, Mo, W, Ru modified titania and ceria oxinitrides and oxides will be carried out. The electrocatalytic activity of these electrodes as cathode components for N2 fixation into NH_3 will be evaluated in the temperature range 200-300 °C and at pressures of 1-100 atm.

Project 8: Two and three dimensional SOFC anode microstructure characterisation

Supervisor
Jacob R. Bowen, jrbo@dtu.dk

- A thorough and detailed characterisation of the standard Risø / Topsoe second generation SOFC anode is required for comparison to solid oxide fuel cells after operation.
- Scanning electron microscopy and image analysis will be used extensively.
- Two dimensional SEM imaging combined with stereological microstructure quantification will be compared to 3D imaging
- 3D microstructure imaging will be performed by focused ion beam serial sectioning and analysed using advanced image processing techniques to calculate important 3D parameters
- The final report is likely to contain intellectual property and parts will remain confidential

Project 9: Improving SEM based X-ray micro tomography resolution

Supervisors
Jacob R. Bowen, jrbo@dtu.dk
Erik Mejdal Lauridsen

- The electron beam of an SEM can be used to generate X-rays from a suitable target for X-ray tomography to create three dimensional microstructure images.
- The X-ray source size strongly influences spatial resolution. The project will explore new target designs to improve resolution.
- The project will also investigate the structure and microstructure of fabrics used in energy devices.
- The final report is likely to contain intellectual property and parts may remain confidential

Project 10: New methods for the alignment of three dimensional electron backscatter diffraction image stacks

Supervisor
Jacob R. Bowen, jrbo@dtu.dk

- Three dimensional microstructure information containing crystal orientation can be collected using conventional 2D EBSD and focused ion beam serial sectioning.
- Reconstructing 3D-EBSD datasets often include alignment errors between slices
- The project will explore new mathematical methods to align data slices
- The final report is likely to contain intellectual property and parts may remain confidential

Project 11: Degradation/passivation of mixed ionic and electronic conducting oxygen electrodes

Supervisor:
Per Hjalmarsson, phja@dtu.dk

Mixed ionic and electronic conducting SOFC-electrodes, such as $La_{1-x}Sr_xCoO_{3-\delta}$, possess high electro-catalytic activity towards oxygen reduction, however, there are still concerns whether these electrodes are durable and robust enough to meet the technological requirements when operated under harsh conditions. This master thesis project will evaluate the effect of potentially hazardous operating conditions on the lifetime of such electrodes using electrochemical and electrical experimental techniques. Additionally, it aims at clarifying the reason for the observed electrochemical degradation by postmortem analysis using techniques such as microscopy and XPS. The student will take part in, and learn from, electrode manufacturing, electrochemical and microstructural characterization and analysis of acquired data. The project focus on experimental analysis but the student is also welcome combine this with theoretical modeling.

Project 12: Intermolecular and Particle-Polymer Interactions in Suspensions for Thick Film Ceramic Processing

Supervisors:
Johan Hjelm (main supervisor), johh@dtu.dk
Debora Marani (co-supervisor)
Michela Della Negra (co-supervisor)

Short Description
Manufacturing of functional ceramic layers for use in energy conversion devices such as high temperature fuel cells rely on specific rheological properties of the suspension carrying the ceramic particles of interest in order to allow well-defined electrode layers to be applied using colloidal thick film techniques such as screen-printing. This study will investigate intermolecular and particle-polymer interactions in solvents of various polarity and in suspensions with so-called associative thickeners (functionalized polymers) added as thickeners.

Detailed Project Description:
The nature of the coating's rheology generally has to satisfy the application properties allowing easy application under high-shear conditions, yet have a high enough viscosity in this region in order to maintain a good film build, or film thickness. Furthermore, the colloidal coating must have a low enough viscosity at low-shear rates in order to exhibit good flow-out and leveling after the high shear of the application, yet still prevent sagging and slumping. Polymers that display strong intra- and inter-molecular interactions in some

cases display associative effects that causes gel-formation at relatively low concentrations, a process that often is reversible. This means that the gel-structure can be broken up, and given the right conditions will re-form within a relatively short period of time. This leads to a time-dependent viscosity of the solution or suspension which can be advantageous in the formulation of inks (suspensions for screen-printing) for high-precision screen-printing applications such as electrode manufacturing.

Intermolecular forces, network formation and strength in polymer solutions of varying polarity will be explored. Conditions under which hydrophobic or hydrophilic interactions dominate are of great interest and will also be addressed. Depending on the outcome of the first and main part of the study, the investigation may be extended to investigation of the effect of adding solid particles coated with surfactants to the polymer solutions. The polymers are expected to display different degrees of interaction depending on the nature of the surfactant coating and the influence of the particles on the rheological properties and the network formation and strength in particle loaded polymer suspensions will be investigated in the latter part of the project.

Rotational rheometry is a very important technique for measurements of flow-properties and viscosity of the different solutions/suspensions. Oscillatory rheometry is a form of mechanical impedance spectroscopy that is very useful for quantifying visco-elastic properties of materials, and these two techniques form the backbone of the experimental investigations to be undertaken.

Main Methods: Oscillatory and Rotational Rheometry, Turbidity Measurements, Laser Diffraction, Particle Size Reduction Techniques (Milling)

Project 13: Studies of colloidal stability in suspensions used to produce elements for solid oxide fuel cells (SOFC) or electrolysis cells (SOEC) by tape casting.
Supervisors.
Michela Della Negra
Trine Klemensø (Co-supervisor)

The purpose of this work consists in producing thin ceramic tapes by tape casting, which will function as electrolyte or electrodes in SOFC or SOEC. For the success of the entire process an optimum control of the properties of the ceramic slurry is required. In fact the mechanical strength, the performance and durability of the final cell strongly depend on the processing procedure. The project will deal mainly with the first step of the slurry preparation, which consists in optimizing the suspension stability, as a good initial dispersion of ceramic powders in liquids is essential for production of high-quality final products with controlled microstructure. In fact agglomerates and inhomogeneities in the dispersion result in poor packing, uncontrolled porosity, and other defects, which can also facilitates initiation and propagation of cracks. This becomes even more complex when dealing with multi-component ceramic slurries, as it happens for SOFC production.
The stability of single and multi-component suspensions will be evaluated by:
Controlling the particle size distribution of ceramic powder in the suspension by light scattering and by comparison with microscopy;
Measuring the zeta potential (property related to the particle surface charge) in the dispersion;
Controlling the sedimentation behavior;
Studying the rheological properties of the suspensions.
These characteristics will be evaluated as effect of powder milling and addition of different type and amount of dispersants. Different solvents could also be considered as well as the pH effect.
The focus of the scientific research will possibly be:

Understanding the effect of mixing 2 types of powders in one system.
Effect of the stabilization on the micro-structure after sintering;
Understanding the effect of the powder properties (structure and/or composition) in the interaction with the dispersant.

Project 14: Fabrication of Solid Oxide Cell Stacks by Ink-jet Technology

Supervisors:
Søren Højgaard Jensen (main supervisor), shjj@dtu.dk
Johan Hjelm (co-supervisor)
Vincenzo Esposito (co-supervisor)

Short description
Solid Oxide Cell (SOC) Stacks are efficient energy converters. With the current manufacturing technology each cell is produced individually and this limits the stack robustness and durability. Manufacturing of the entire SOC stack by Ink-jet printers is a new and interesting research area. The project goal is to write a printer driver to enable a 2D printer to print the first preliminary SOC stack and to investigate the performance of the printed stack using impedance spectroscopy and electron microscopy.

Detailed Project Description:
In a fuel cell hydrogen and oxygen are converted into electricity with heat and water as by-products. The process is not an ordinary combustion with a flame but a direct transformation of chemical energy into electrical energy. This makes it possible to achieve very high conversion efficiency. It is also possible to reverse the cell process to make it work as an electrolyzer, using electricity and water to make hydrogen and oxygen.
A promising way to store wind and solar electricity is by electrolysis of H_2O and CO_2 using solid oxide electrolysis cells (SOECs) to produce synthetic hydrocarbon fuels that can be used in existing fuel infrastructure. Solid Oxide Cell (SOC) stacks are normally assembled at room temperature, one cell at a time. This imposes that the various layers of the stack must be pressed together during operation to establish a good electric contact between the layers. Due to the heat generated in the SOCs the temperature in usual stacks can vary more than 100 ˚C. The induced thermal stress limits both the robustness and lifetime of the stack. Ink-Jet printing of SOC stacks could help solving these problems.
The design strategy is to produce one layer of the stack at a time with a printer, also known as additive layer manufacturing (ALM). The layers should be made with inks containing sub-µm-size particles of seal, pore former, interconnect and electrolyte materials. After printing, the stack is taken to a furnace and sintered at high temperature at a reducing atmosphere to assure good mechanical and electrical stability during operation. Dedicated 3D printers are very expensive and this hinders mass production of SOC stacks with Ink Jet technology. This project aims to use a low-cost consumer-end 2D printer to circumvent the obstacle. The low-cost printers have sufficiently high x-y resolution to allow formation of holes for - and sealing of - gas channels in the various components of the SOCs. In order to fully enable the printer for printing of ceramic layers it is necessary to develop a custom printer driver. The project goal is to write the printer driver, print the first preliminary SOC monoliths and investigate the performance using impedance spectroscopy and post mortem analysis methods.
Main Methods: Electrochemical Impedance Spectroscopy, Electron Microscopy, Energy Dispersive X-ray Spectroscopy and various other characterization techniques depending on the outcome of the project.

Project 15: Enhancing the physical robustness of Solid Oxide Cells (SOCs)

Main Supervisor: Tânia Ramos (Senior Researcher)
Co-Supervisors: Bhaskar Sudireddy (Researcher)
and Mogens Mogensen (Research Professor)

Short description

Key parameters for the success of Ni-cermet support layers include inhibited microstructural degradation, mechanical strength, chemical stability and compatibility. This project aims to contribute to the improvement of their physical robustness, through tailoring of both microstructure and composition. The use of partially stabilised zirconias (PSZs), other than yttria-stabilised (YSZ), is not commonly seen in SOCs but very much envisaged for this project. In addition, Ni-ceramic ratios and porosity levels must be also exploited, in the search for a compromise between robustness and performance.

Extended description

Strategies for generation of anode support materials and structures of improved robustness will be explored. This involves tailoring of the microstructure and composition of the support to improve its physical robustness, *e.g.* inhibition of Ni-particle growth and improved mechanical strength, whilst maintaining or improving its chemical stability and compatibility during operation.

Improved robustness may be obtained by changes of the microstructure and/or by use of alternative materials, e.g. MgO and/or CeO_2 doped ZrO_2. Either way, definition of optimum ratios, % porosity, pore shape/distribution, and thickness must be defined in a compromise between robustness and performance. In addition, the support structure sintering profile must allow for electrolyte densification, and not induce detrimental mismatches during de-binding and sintering.

This project may therefore involve some of the following subjects:

- Materials survey and recipe formulation;
- Production of various tape-cast anode supports;
- Compositional and microstructural optimisation;
- Characterisation pre and post reduction;
- Mechanical and electrochemical testing;
- Component integration (depending on time)

The main characterisation techniques may include:

- SEM, EDS and low-voltage SEM;
- Electrochemical impedance spectroscopy;
- Hg intrusion – porosity measurements;
- Particle size measurements;
- Dilatometry and optical dilatometry;
- XRD.

Project 16: Understanding and optimising the low temperature reduction of Ni/(Sc)YSZ SOFC anodes

Main Supervisor: Tânia Ramos (Senior Researcher), tara@dtu.dk
Co-Supervisors: Anne Hauch (Senior Researcher)
And Johan Hjelm (Senior Researcher)
Supporting project: Smart grid ready SOFC

Short description

The initial reduction procedure of NiO $\rightarrow$ Ni/(Sc)YSZ cermet SOFC anodes generates most of the required porosity, impacting also Ni grain sizes, Ni percolation and possibly Ni-ceramic adhesion properties. Recent MSc work at our department has clearly shown its importance, bringing to light interesting differences between the two compositional systems (Y or ScY). This project aims to further understand the parameters ruling such differences, not only to tackle them and optimise a reduction procedure suitable for each system, but to deliver the best possible initial microstructure. This should enable a good start for the envisaged long life of a working SOFC.

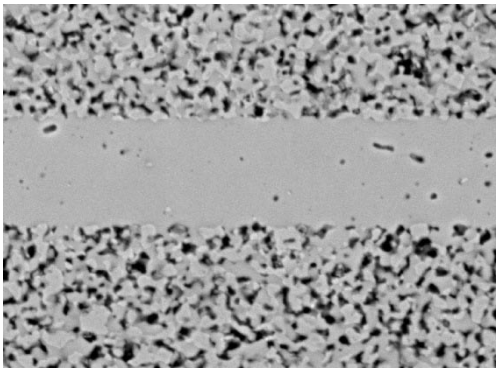


Figure 1. Scanning electron micrograph of Ni/ScYSZ SOFC anodes, in a symmetric cell configuration, that have exhibited good electrochemical performance.

Extended description

Although many times neglected, the initial reduction of Ni-based cermet SOFC anodes is an important step. As shown by a recent MSc work conducted at our Department[1], failure to establish a good initial microstructure may decrease, or even completely stop, electrode performance. Parameters such as temperature and steam content in the fuel gas seemed to play an important role. In addition, Ni/ScYSZ and Ni/YSZ based electrodes also exhibited different behaviours for similar reduction parameters, especially when reduced at lower temperatures (≤ 850°C).

This project will focus mainly on reduction at low temperatures, in an attempt to gain further understanding of which and how parameters, such as reduction atmosphere, affect the creation and maintenance of microstructures that can translate into excellent initial performances. Knowledge will give fuller control, and increase the ability to tailor the reduction conditions in order to maximise the potential of the different, technologically relevant SOFC anode compositions.

Therefore, the project may involve all or some of the following lines:

- Electrochemical testing of Ni/YSZ and Ni/ScYSZ SOFC anode materials;
- Microstructural characterisation: SEM, low voltage-SEM and possibly TEM
- Surface area and porosity measurements

- Image analysis
- Thermogravimetric analysis
- Production of modified symmetric cells.

1) Søren Ebbehøj, "Enhancing the performance and the stability of Ni/(Sc)YSZ electrodes - *A study of the in-situ reduction of Ni/(Sc)YSZ-cermet anodes ",* MSc Thesis, Risø DTU, 2011

Project 17: Infiltrated Ni-(Sc)YSZ SOFC anodes for improved carbon and sulfur tolerance

Main Supervisor: Tânia Ramos (Senior Researcher)
Co-Supervisors: Christopher Graves (Researcher)
Supporting project: Smart grid ready SOFC

Short description

The quest for SOFC anodes with better performance and tolerance is on-going. From this search, is it now known that the intolerance of Ni-cermets towards sulfur and carbon can in principle be mitigated, or even eliminated, by addition of other materials to the electrode. Also, when certain materials are added as nanoparticles, the electrochemical performance of the Ni-cermet electrode can in general be improved. What are the best materials and how they behave are still open questions. For this reason, this project involves systematic testing of infiltrated Ni-cermets, as means to identify potential materials for enhanced tolerance, and gain fundamental understanding on the influence of infiltrated nano-particulate coatings.

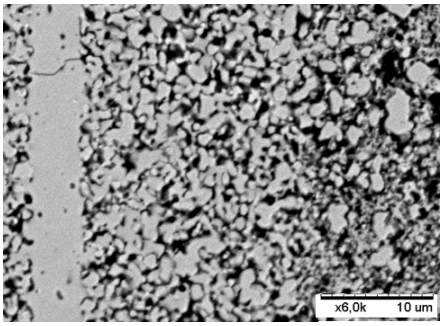


Figure 1: Scanning electron micrograph of a Ni/ScYSZ SOFC anode and Ni/YSZ support layer, pre-reduced and ready for infiltration.

Extended description

The most common SOFC anode, a composite of nickel and yttria-stabilized zirconia (Ni-YSZ), is highly electro-catalytic for electro-oxidation of hydrogen- and carbon-containing fuels, as well as for electrolysis of steam and carbon dioxide. However, Ni is also an excellent catalyst for carbon deposition reactions (Boudouard reaction and hydrocarbon pyrolysis reactions) and it strongly adsorbs sulfur. Carbon and sulfur therefore block reaction sites, rapidly deactivating the electrodes. In some cases the poisoning is reversible, while in other conditions Ni can irreversibly react with the deposited carbon or adsorbed sulfur, even damaging the mechanical integrity of the electrode.
It has been reported that this known intolerance of Ni towards sulfur and carbon can be mitigated or even eliminated by adding other materials to the electrode, in order to modify its surface chemistry. Also, when certain materials are added as nanoparticles, the electrochemical performance of the Ni-based electrode can be improved in general. At DTU Energy Conversion, we have an ongoing project in infiltration of such materials into state-of-the-art porous Ni-based SOFC anodes to produce nanoparticulate coatings on the surfaces of the porous structure. The aim of this project is to provide a

systematic evaluation of the potential of different additives as tolerance enhancers, and gain further understanding of their properties as nano-particulate coatings.

The main work lines involve:

- Microstructural analysis: encompasses surface area (BET)/porosity measurements on infiltrated and non-infiltrated electrodes and scanning electron microscopy (SEM) of infiltrated electrodes;
- Phase analysis: XRD analysis of bulk samples composed of the same materials as the infiltrated electrodes (Ni-SZ + infiltrate material)
- Electrochemical characterization: testing of infiltrated cells in a symmetric configuration, using electrochemical impedance spectroscopy (EIS), under a variety of operating atmospheres (sulfur and carbon containing). Best additives to be considered further for full cell testing.

Project 18: In situ surface study with high temperature scanning probe microscopy

Supervisors:
Mogens Mogensen
Karin Vels Hansen

In situ studies are becoming more and more frequent because they give information on a system when it is working. The project is experimental and includes surface studies with a unique high temperature scanning probe microscope which can reach the temperature relevant for solid oxide fuel cell operation. This enables a study of the electrical surface properties with time and as response to e.g. atmosphere changes. Surface properties are determining for the electrochemical performance of solid oxide fuel cells. The study will focus on relevant materials. Conventional ex-situ techniques such as scanning electron microscopy will be used to characterize the microstructures.

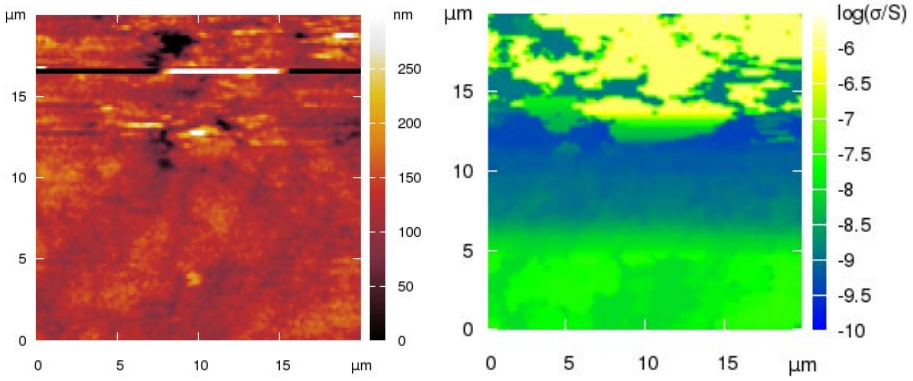


Figure 1. Example of topography and surface conductivity obtained during in situ reduction of NiO-YSZ at 500 °C.

Project 19: Protective coatings for the improvement of corrosion resistance of porous steels for Solid Oxide Fuel Cells

Supervisor: Sebastian Molin (sebmo), PostDoc
Co-supervisor: Nikolaos Bonanos (nibo), Senior Scientist

Solid Oxide Fuel Cells are energy converting devices that allow for the highest efficiencies of energy conversion and thus have gained gained a considerable attention of the scientific and industrial groups.
Among the obstacles in the development of this technology are degradation phenomena and high price of materials and processing. During recent years one of the research trends include incorporation of cheap metallic alloys into both interconnect and into the supporting structure of cells, so that expensive ceramic materials are replaced with cheap alloys with relatively simple processing.

Due to the large specific surface area of porous alloys, their corrosion at high temperatures might limit the lifetime of fuel cells. Corrosion causes lowering of the electrical conductivity and can also lead to blocking of pores, that will limit gas access to electrodes. In order to reduce corrosion rates protective coatings are used. These can be based for example on the so called reactive elements with very high oxygen affinities (i.e. Y, Ce, La, Gd). Coatings will be prepared by impregnation of metalooorganic precursors and subsequent heat treatment. Effect of coating composition and loading will be evaluated by determination of high temperature corrosion properties. Mass gain of samples and porosity changes during cyclic oxidation experiments will be measured. Oxide compositions will be evaluated by x-ray diffractometry (XRD). After oxidation experiments samples cross sections will be analyzed by scanning electron microscopy (SEM) and energy dispersive x-ray analysis (EDX).

It is anticipated that the developed coatings will decrease the corrosion rate of porous alloys significantly.

The research group at DTU Energy Conversion has a broad experience in fabrication of metal supported Solid Oxide Fuel Cells and in corrosion testing of interconnects and porous supports. The student will gain hands-on experience with materials processing and modern analytical techniques in an international research group.

Project 20: Evaluation of Nb-doped SrTiO3 SOFC anodes modified with other transition metals (W, Mo, Fe, Cr, Cu)

Main Supervisor: Bhaskar Sudireddy, Researcher
Co-Supervisor: Tânia Ramos, Senior Researcher
Supporting project: SCOTAS-SOFC (EU)

Short description
The search for SOFC anodes with increased tolerance to redox cycles, sulphur containing fuels and carbon deposition, has been a quest of many researchers over the years. In addition to tolerance, alternative anode materials must be capable of performing to a level close to that of Ni-based cermets. SrTiO3 based materials, e.g. Nb-doped SrTiO3 (STN), when infiltrated with suitable electrocatalysts have the potential to provide just that. This project aims to assess and exploit further the potential of STN SOFC anodes both by co-doping and/or

infiltration of other transition metals, e.g. Mo, W, Fe, Cr and Cu. Powder synthesis, infiltration, microstructural, chemical and electrochemical characterisation are envisaged.

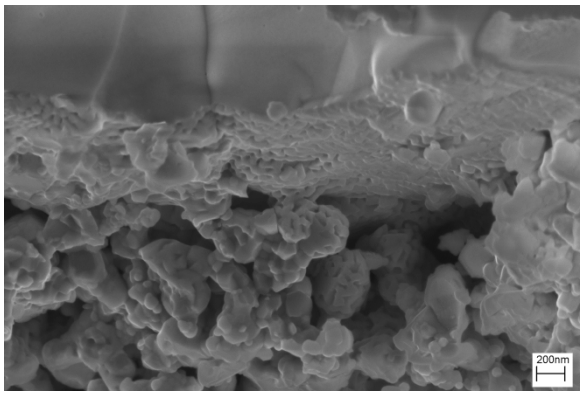


Figure 1. Scanning electron micrograph of a Ni/CGO infiltrated STN porous backbone.

Extended description
In addition to Nb, the B-site of SrTiO3 may also be successfully substituted with other transition metals, e.g. W, Mo, Fe and Cr, and still form a single perovskite phase. Since W and Mo can be reduced to +4 oxidation states, they will probably have higher affinity to occupy the B-site when compared to the Nb on STN. In a co-doping situation, Nb may be forced to leave the B-site. On the other hand Fe and Cr, with a +3 oxidation state, may introduce oxygen vacancies into the titanate, and thereby by some ionic conductivity. The impact of co-doping and the expected modifications to the surface of STN may have interesting consequences to its performance and robustness, particularly in the presence of infiltrated nano-electrocatalyst particles. In addition, the interaction of the "forced out" Nb with other infiltrated transition metals is of particular interest for the electronic and catalytic properties of STN based electrodes.
This project may therefore involve all of some of the following lines:
Powder synthesis, sintering of materials;
Fabrication of electrodes;
Infiltration of electrodes;
Electrochemical testing of co-doped and/or infiltrated cells in a symmetric configuration;
Microstructural (SEM and/or TEM), chemical and structural characterization (EDS, XRD)

Project 21: CERMAC: Cost Efficient Regenerative Metal-Hydride Air Cell.

Supervisor
Didier Blanchard.

The objective is to develop a novel hybrid system for efficient conversion of sustainable chemical fuels to electricity, which combines the efficiency and flexibility of fuel cells (FC) with the regenerative properties and stability of nickel metal hydride batteries (Ni-MH) and minimizes the dependence on rare earth metals. An AB_5 metal hydride catalyst optimized by nano-structuring and coating to achieve high electrical power density and stability, will be used for the hydrogen electrode (anode) instead of expensive Pt-based catalysts. The intrinsic

hydrogen storage capacity eliminates the challenges associated with FC start-up and interrupted fuel supply by working as a rechargeable battery. The oxygen electrode (cathode), consisting of a bi-functional catalyzed air electrode (perovskite oxides) will lower the weight of conventional Ni-MH electrodes, with the bonus of using oxygen from air, thus increasing the energy density of the cell. A laboratory prototype will be built and tested for cycling stability, targeting power densities of 100 mW/cm^2, current densities of 200 mA/cm^2 at significant reduced prices. The project, combining state *of the* art materials and *in-situ* experimental techniques, will enable the applicant to collaborate with internationally recognized experts (Prof. Tony Spassov from Sophia University and Prof. Dag Noréus from Stockholm University).
The project will bring valuable knowledge for the development of high power density batteries and ultimately help solve the main technological challenges facing commercial success of Electrical Vehicles. It is divided in three parts:

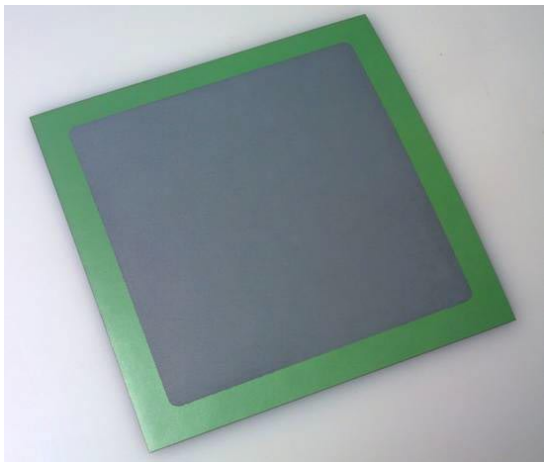
- Test and characterizations of the AB_5 metal hydrides optimized by nano-structuring and nano-coating. Synthesis in collaboration Prof. Tony Spassov. Study on the stability of the hydrogen storage properties upon cycling.
- Synthesis and characterization of the perovskites oxides (Synthesis at DTU Energy Conversion).
- Assembly and test of the cells (electrodes fabrication in collaboration with Prof. Dag Noréus)
    - Testing of the electrodes electrocatalytic activities in half-cells set-up.
    - Test of the full cells.

Project 22: Novel techniques of thermo-mechanical characterization for lifetime prediction in glass-ceramic sealings

Supervisors:
Dino Boccaccini (dinb@dtu.dk)
Ragnar Kiebach (woki@dtu.dk)

DTU Energy Conversion and Storage and the industrial partner Topsoe Fuel Cell A/S have successfully been using commercially available glasses for the sealing of stacks which operate at 750 - 800°C. Concurrently, Risø DTU has been focused in the development of a new generation of SOFCs of glass-ceramic sealings which should be able to operate at lower temperatures with increased efficiency and lifetime. Currently, new glasses have been developed to obtain a better match of the thermo-mechanical properties between sealant and the adjacent stack components and to tailor the crystallization behavior of the glass. However, at the current development stage, it is unknown how these new glass sealings can withstand the thermo-mechanical stresses arising during service life of the stack. Hence it is of primordial importance the finding of reliable methods for

the characterization of thermo-mechanical properties and to study the influence of ageing in these properties to permit to estimate lifetime.



Project Content:
The aim of the master thesis is to develop a lifetime prediction method for glass sealings used for SOFC cells. Usually, in service, glass ceramic sealings are subjected to thermo-mechanical stresses that could lead the sealings to leak over time. At the state of art conditions, there is no a proven reliable method able to predict lifetime of this SOFCs components based on simulation of the service life conditions. The Thermo-mechanical analyzer(TMA) by NESCHT s a newly developed instrument that can analyze the thermo-mechanical properties of materials. The behavior of materials under creep, mechanical and thermal fatigue conditions can be completely studied and modeled at laboratory level and the feasibility of these models to estimate lifetime of materials could be assessed.
The following characterization methods will be used by the master student in this project: *Thermo-mechanical Analyzer (TMA), Advanced Electron Microscopy/Energy Dispersive X-ray Spectroscopy (SEM/EDS), Thermal analysis (modern Thermogravimetric/Differential Thermal Analyzer* (DTA/TG), *Differential Scanning Calorimeters* (DSC) and *in-situ optical dilatometry*.

Project 23: Novel Sealing Strategies for Metal Supported Solid Oxide Fuel Cells

Supervisor
Ragnar Kiebach, woki@dtu.dk, tel. (+45)-4677-5624.

Background:
According to the Danish Energy Plan 2050 up to 50% of the electricity must be generated from renewable energy sources, mainly by wind power. For this scenario to be viable, a considerable capacity for power storage and power conversion must be established. In this context, SOFC technology can be used to convert biogas or hydrogen into clean electricity when power demand exceeds production.
Risø DTU has been involved in the development of SOFCs for several years and is among the world leading institutes in this area. The latest generation of SOFC uses “metal supported cells” (Fig. 1). These cells are expected to offer several potential advantages over conventional anode (Ni-YSZ) supported cells (e.g. increased

resistance against mechanical and thermal stresses and a reduction in material costs). The novel cell design shows a promising performance and durability at a broad range of temperatures and is especially suitable for intermediate temperature operation below 650 °C.

On drawback at the current development stage is that only little is known about how these new cells can be joined/sealed to other parts.

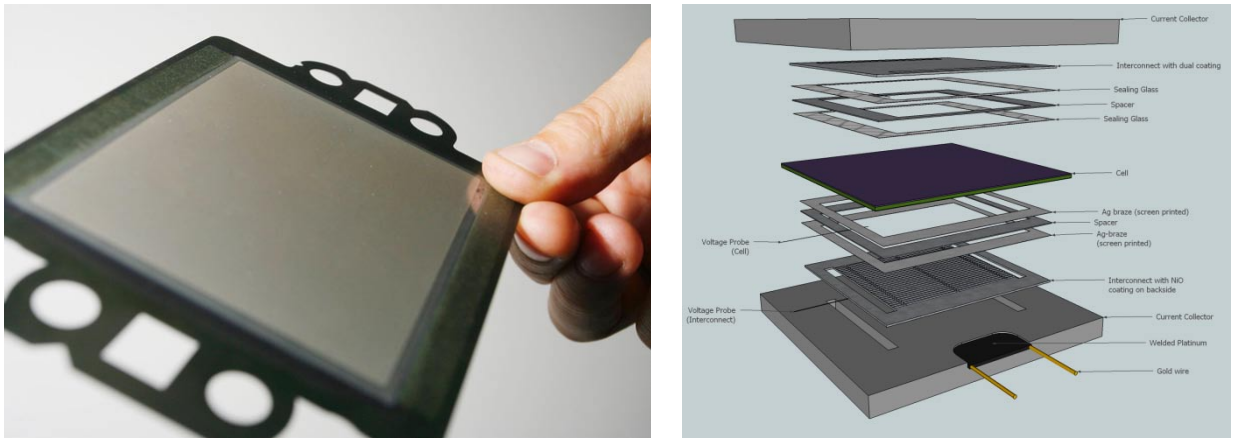


Figure 1: Metal supported cell and test setup for SOFC including sealing

Project Content:

The aim of the master thesis is to develop a sealing solution for metal supported SOFC cells. Usually, glass or Ag based brazes or used to obtain gas tight joints between the cell and other stack components. Existing solution for conventional cells cannot be used here, since the materials may not be compatible and the operation temperature is different. Therefore new seals must be developed. Here, possible glass/glass-ceramics and brazes suitable for low temperatures will be characterized and tested. The main focus will be on the characterization of the microstructure of interface of the metal supported and the glass as well as on studying the chemical reaction between the used materials at high temperatures.

The following characterization methods will be used by the master student in this project: Advanced Electron Microscopy/Energy Dispersive X-ray Spectroscopy (SEM/EDS), Thermal analysis (modern Thermogravimetric/Differential Thermal Analyzer (DTA/TG), Differential Scanning Calorimeters (DSC) and in-situ optical dilatometry. The most promising materials will be selected for actuial leak tests with opaating SOFC cells.

Project 24: High performance SOFC Anodes Based on Infiltration of Ni-$Ce_{0.8}Gd_{0.2}O_2$

Supervisor:
Ragnar Kiebach, woki@dtu.dk, tel. (+45)-4677-5624.

Background:

Solid oxide fuel cells (SOFCs) are electrochemical devices that convert chemical energy to electrical energy with high efficiency. A relatively high operation temperature (600 – 1000 °C) makes the SOFCs suitable for operation using a variety of fuels (i.e. hydrogen, hydrocarbons, Biogas). Conventional SOFCs use Ni as anode material due to its high catalytic activity for fuel oxidation and high electronic conductivity. It is most frequently used in the form of a composite with yttria stabilized zirconia (YSZ) in order to increase the Ni-YSZ contact area for higher anode efficiency and obtain good connection with the electrolyte (Figure 1a). These composites are generally fabricated by mixing YSZ and NiO powders and co-sintering at elevated temperatures (1200 – 1350 °C) followed by in-situ reduction. One major disadvantage of these anodes a loss of percolation (loss of contact, Fig. 1b) of Ni particles during operation, which leads to decreased performance.

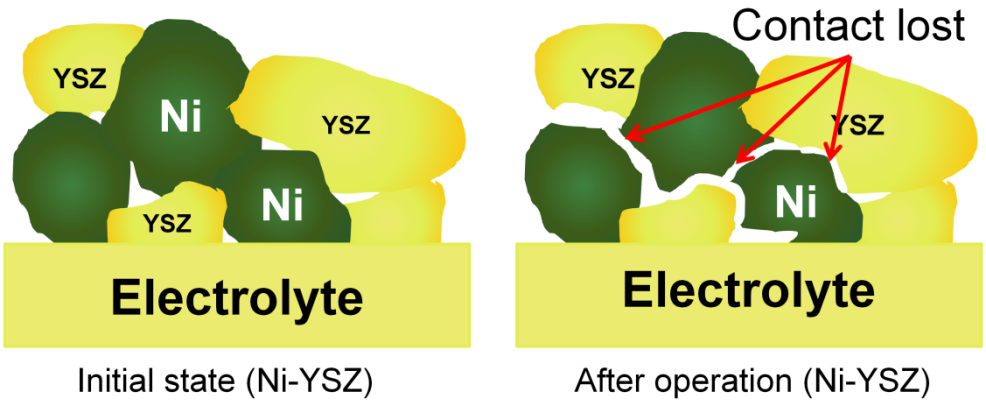
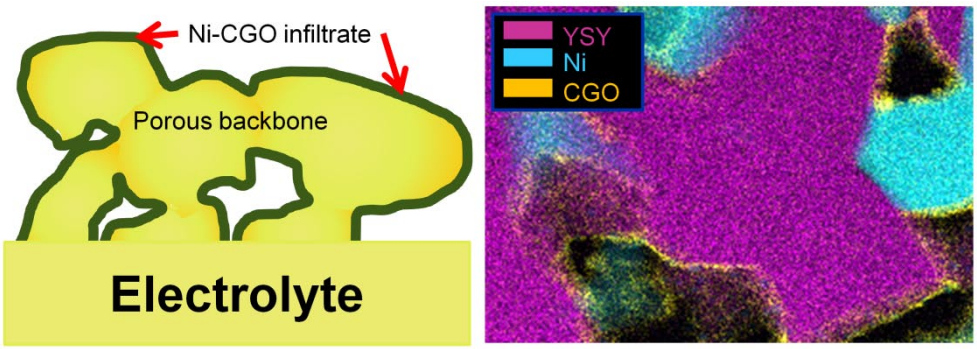


Figure: Degradation of Ni-YSZ Anodes

Objectives:

The goal of the diploma/master thesis is to develop a fabrication route for more stable and better performing SOFC anodes using infiltration techniques. Infiltration of the catalytically active phase into porous YSZ backbone (Fig. 2) has been reported as a prospective way to fabricate SOFC electrodes with high surface areas. This technique has been suggested as a promising route to fabricate stable Ni-YSZ anodes. In this project Ni-$Ce_{0.8}Gd_{0.2}O_2$ (Ni-CGO), a promising new anode composite material, will be used. The main focus will be on the characterization of the microstructure of the infiltrated species as well as on studying the relation of microstructure and the electrochemical performance.

The following main characterization methods will be used by the master student in this project: *Advanced Electron Microscopy/Energy Dispersive X-ray Spectroscopy (SEM/EDS), X-Ray Powder Diffraction (including high temperature in-situ investigations),* and *BET-analysis (surface area analysis)*. Also *high resolution transmission electron microscopy* (HR-TEM) will be used for nanoparticle characterization. The most promising materials will be selected for electrochemical testing in real SOFC applications (cell or stack level).



Backbone infiltrated with Ni-CGO

TEM/EDS image of Anode infiltrated with Ni-CGO

Figure 2: Infiltration of Ni-CGO – Concept and example

Project 25: Test of components of a carbon-oxygen battery

Supervisors
Chris Graves cgra@dtu.dk
Mogens Mogensen momo@dtu.dk

Background:

We are working on a promising new type of electrical energy storage device, a rechargeable carbon-oxygen battery. The battery electrochemically converts CO_2 into solid carbon particles and O_2 in charge mode and the reverse net reaction occurs in discharge mode. Because solid carbon is a highly energy dense material, the total energy density can be a factor of 10 higher than existing Li-ion batteries and much higher than hydrogen energy storage.

The following reactions take place during charge mode (and the reverse take place in discharge mode):

(1) $2\ CO_2$ + electricity + heat → $2\ CO + O_2$ (CO_2 electrolysis)

(2) $2\ CO \rightarrow C + CO_2$ + heat (carbon deposition by the catalytic Boudouard reaction)

By coupling the two reactions, high energy storage efficiency can be obtained by taking advantage of the near-zero entropy change of the net reaction (CO_2 + electricity → $C + O_2$). The theoretical maximum roundtrip electricity-to-electricity efficiency is 100% for this storage chemistry (compared with only 70% for $H_2O \leftrightarrow H_2 + O_2$). In the battery, the reactions are coupled by carrying them out consecutively, but in close proximity, by (a) careful choice of different materials for the electrodes (which do not catalyze carbon deposition) and the carbon deposition sites, and (b) designing the cell/stack/system to facilitate efficient heat transfer between the two reaction sites.

Purpose of the Master project:

The aim is to prove the technical coupling of the electrochemistry with the Boudouard reaction. The most crucial is to prove that we can get a reasonable high overall reaction rate. This is needed before we can go on with designing a full battery system.

The work of the Master project

The work for this project entails (1) study of performance and stability of electrodes in miniature cells in CO/CO_2 atmospheres with cathodic polarization, (2) measurement and modeling of Boudouard reaction kinetics in small tube reactors under battery relevant conditions, and (3) if possible take part in testing of 5x5 cm cells produced in other projects if they appear to be reasonably stable at the high (e.g. 90 %) pCO_2 required in the battery negative-electrode chamber.

Project 26: Advanced Electrochemical Testing of Solid Oxide Cell degradation

Supervisors: Søren Højgaard Jensen (main supervisor), Chris Graves (co-supervisor), Anne Hauc (co-supervisor)

Project description (5-line summary)

Solid Oxide Cell (SOC) Stacks are efficient energy converters. However, the SOC durability does not fully meet commercial requirements of long term stability. Various processes may lead to degradation of SOCs and one way to investigate these processes is by electrochemical impedance spectroscopy. The project aim is to quantify and characterize the degradation processes, by applying an advanced test method involving analysis of differences in impedance spectra recorded during SOC operation.

Detailed Project Description:

In a fuel cell hydrogen and oxygen are converted into electricity with heat and water as by-products. The process is not an ordinary combustion with a flame but a direct transformation of chemical energy into electrical energy. This makes it possible to achieve very high conversion efficiency. It is also possible to reverse the cell process to make it work as an electrolyzer, using electricity and water to make hydrogen and oxygen.
A promising way to store wind and solar electricity is by electrolysis of H_2O and CO_2 using solid oxide electrolysis cells (SOECs) to produce synthetic hydrocarbon fuels that can be used in existing fuel infrastructure.
The SOC consists of two electrodes on either side of an electrolyte. Electrochemical impedance spectroscopy can be used to investigate the electrode processes that govern the performance and durability of SOCs. In order to quantify and characterize the processes, an equivalent circuit is used to model the SOC impedance spectra (IS). Unfortunately, the optimal equivalent circuit is often unknown and to complicate matters further, several processes contribute to the SOC impedance - making detailed process characterization difficult. By applying small changes in the gas composition during operation of a SOC and measure the change in the impedance spectra it is possible to distinguish which of the electrodes that degrades.
The project aim is to measure, analyze and model a series of IS measured during operation of an SOC to improve the overall modeling accuracy and quantify the electrode degradation.

Main Methods: Electrochemical Impedance Spectroscopy, Electron Microscopy, Energy Dispersive X-ray Spectroscopy.

Project 27: New electrocatalysts for effective water splitting in alkaline solutions.

Supervisors: Aleksey Nikiforov and Jens Oluf Jensen

One of the most important aspects of today's society is an energy question. The interest to renewable energy sources has increased significantly during last decades. Therefore, the amount of research and investments in this sector continues to grow these days. One of the important targets for the Danish energy sector is to consist of mostly of renewable energy in the grid by year 2050. This should include such important technologies like extraction of energy from solar and wind sources. However, the renewable energy sources are not available continually, as sun does not shine at night and wind does not blow all the days. Therefore, one of the crucial aspects will become the storage of energy, extracted from renewable sources. Water electrolysis is an elegant solution of this problem, as the produced renewable energy can be used to split water to hydrogen and oxygen at the peaks of energy availability. Further hydrogen can be used either directly in fuel cell, or be combined with CO_2 (contained in ambient air) for production of more common fuels, like methane. Alkaline water electrolysers present an available solution for renewable energy storage. These days one of the perspective types of water electrolysers is under development, so-called, "Zero-gap" alkaline systems. Those systems would combine advantages of PEM and alkaline systems. Highly active electrocatalysts for such systems are under high demand and development of them is ongoing at Proton Conductors section in Lyngby campus.
Several ideas can be worked out to speed up the development:

1.) Syntesis of electrocatalysts by alternative methods for archiving high surface area.
2.) Building up a cell for long-term test of electrocatalysts in working electrolyser.
3.) Standard Operating Procedures (SOPs) developing and implementing for screening of the most perspective materials.

For further information please contact Aleksey Nikiforov nava@dtu.dk or Jens Oluf Jensen joj@dtu.dk

Project 28: Construction and electrocatalytic activity for medium temperature energy systems.

Supervisors: Aleksey Nikiforov and Irina Petrushina

Recently, intermediate temperature solid state fuel cells and electrolysers, which are operated in the temperature range of 150-300 °C, attracted widespread interest because of their higher CO tolerance, faster electrochemical reaction kinetics, simpler thermal and water management, and what important, because of high probability of use of non-platinum catalysts, as compared to the polymer membrane fuel cells. Because the working temperatures of intermediate temperature fuel cells (ITFCs) are lower than that of solid oxide fuel cells (SOFCs), ITFCs would allow the use of oxidation resistant metallic alloys or even plastics as interconnect materials. They would also reduce the operating cost, increase the durability and extend service life time.
Several ideas can be worked out to speed up the development:

1.) Test of candidate materials in the system, simulating conditions of intermediate temperature water electrolysers
2.) Design and test of a cell for high temperature test of the powders.

For further information contact Aleksey Nikiforov nava@dtu.dk or Irina Petrushina irpe@dtu.dk.

Project 29: Organic synthesis of light harvesting materials for polymer solar cells

Short description

Rational design and development of novel conjugated organic materials that can match the solar spectrum more efficiently can result in better energy harvesting in polymer solar cells and consequently enhance the power conversion efficiency towards commercial viability.

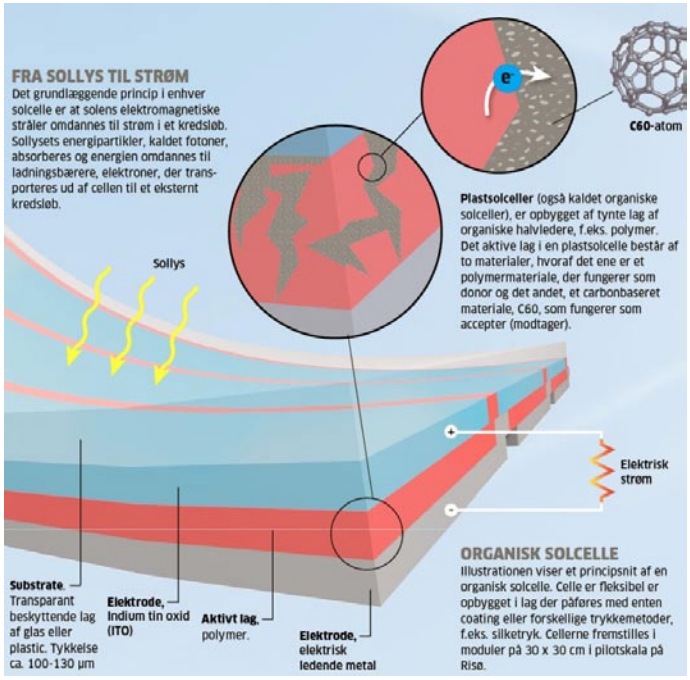
Detailed description

Polymer solar cells (PSCs) offer an environmental friendly alternative to the fossil fuels which our energy society today depends on. During the past two decades research in the field of PSCs has increased tremendously focusing on performance parameters such as efficiency, stability and processing of large devices by methods suited for mass-production.

Most of the increase in efficiency of PSCs is due to the development of new types of polymers with alternating donor and acceptor groups. Their absorption profile can be tuned to match the solar spectrum in order to extract the energy efficiently. The possible donor acceptor structures and combinations are far from exhausted and the goal of this project is to further advance the energy harvesting properties by design and synthesis of novel conjugated polymers of this type. Just as important but less explored is the stability of the organic materials and their processability in large scale roll to roll (R2R) fabrication. These parameters can be studied by fabrication and characterization of PSC devices based on the synthesized materials.

The student will be an integrated part of a larger group that focuses on development of photo-active materials for large scale production of PSCs.

The student will have the possibility to work with:
Monomer synthesis and polymerizations involving a wide range of chemical reactions (e.g. Grignard, brominations, organolithium chemistry, Pd-catalysed cross-couplings).
Characterization of organic compounds using ex: NMR, SEC, UV-vis, AFM etc.
Fabrication and characterization of PSCs
Stability testing of PSCs



Prerequisites

-Practical experience with organic synthesis.
-Motivation.

Supervisors

Eva Bundgaard, E-mail: EVBU@dtu.dk
Martin Helgesen
Jon Carlé