Transition metal oxide electrocatalysts for H_2O splitting

Transition from fossil fuels to renewable energy sources requires efficient storage methods because of their intermittent nature (sun, wind for instance). A promising approach is to convert this energy into a chemical form by using the generated electricity to perform water electrolysis, also known as water splitting, since from water, hydrogen (H_2) and oxygen (O_2) are generated. This hydrogen can be converted back into electricity later or used as a feedstock for chemical processes. The efficiency of water electrolysis depends on the water conversion, and therefore, on the materials used as electrodes where the reactions take place. To accelerate the reactions, catalyst materials have to be used. Transition metal oxide (TMO)-based catalysts are particularly interesting for application in (alkaline) water electrolysis.

In the group, we are investigating electrodes fabricated by atomic layer deposition (ALD). The electrodes are basically made of a support (substrate) coated with an ALD coating (thin film, < 100 nm), the electrocatalyst. This technique enables to tune various parameters of the films such as the chemical composition and crystallographic orientation, thereby modifying their properties. This then allows to study the link between the material properties and the electrochemical behaviour of these electrocatalysts. We are currently working on the following topics:

TMO alloys as OER electrocatalyst
Alloys of cobalt-, nickel- and iron oxide show great promise for application as oxygen evolution reaction (= one half-reaction of the water splitting process) electrocatalysts. Upon alloying, there are large changes in their material properties, such as crystal structure, oxidation states and conductivity. In this research we study how these changes in material properties affect both the electrocatalytic activation and performance of these films. In recent work[1], we have for example seen that cobalt nickel oxides can transform from poorly conductive films to semi-metallic films depending on the chemical composition. We furthermore show that these changes in electrical conductivity also largely affect the electrocatalytic performance of these films. In this project you would work on systematic investigations on the influence of chemical composition on both the material properties and the electrocatalytic OER performance of (alloys of) transition metal oxide thin films.

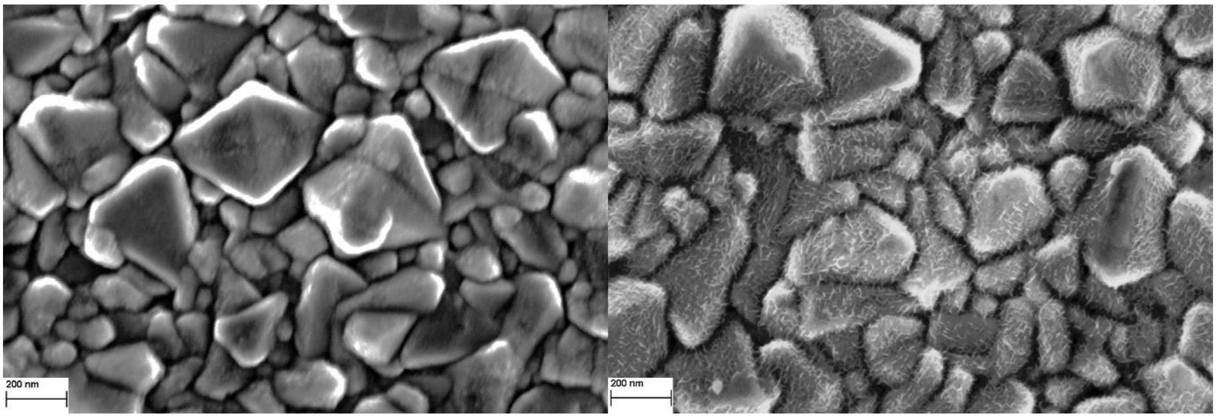

Figure 1: Scanning electron microscope images of a cobalt nickel oxide thin film a.) as deposited, b.) after use as a water electrolysis catalyst

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ALD of electrocatalysts for H_2O splitting

The project's primary objective is to develop highly efficient electrocatalysts for water splitting using ALD, which can lead to improved energy efficiency and sustainable hydrogen production. The collaboration with the Dutch Institute for Fundamental Energy Research (DIFFER) provides an opportunity to conduct in-depth electrochemical characterizations and focus on the electrochemical properties of the developed catalysts.

The first phase of the project comprehensively investigates the impact of different ALD process parameters on the materials properties and electrocatalytic activity of nickel oxide (NiO) films, a highly efficient and cost-effective material, for the O_2 evolution reaction (OER). We examine plasma-assisted and thermal ALD NiO recipes, with a focus on the prolonged electrochemical activation process and its effects on their electrocatalytic performance. The results provide deeper insights into the link between ALD process parameters and electrocatalytic efficiency, paving the way for further development of NiO-based electrocatalysts for OER using ALD.

In parallel to the above work, the second phase of the project is expected to begin in mid-2023, focusing on developing a potential electrocatalyst for the H_2 evolution reaction (HER), the other half-cell reaction in water splitting. The project offers students an opportunity to work in a cutting-edge research field, gain hands-on experience with advanced techniques and equipment, and receive guidance from leading experts at the PMP group (TU/e) and DIFFER.

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Other atomic layer deposited TMOs for water splitting

Due to the cost and scarcity of several elements, e.g. noble metals and possible toxicity issues of already found alternatives, other materials are under research. In this context, we are developing other electrocatalysts: manganese oxides (MnO_x). Since it is a new project, the ALD process has to be proceed and characterized (e. g. chemical composition, crystallinity, morphology). On the other hand, its catalytic effect for oxygen evolution reaction (OER, water to O_2) will be assessed- as well as its stability.

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