Final report for research project "Neutron scattering studies of hydrogen in fuel-cell relevant materials" (ref. 19-553)

Summary of the project - This research project focused on the application of the technique neutron reflectivity (NR) to study the nature of the protective surface oxide layer on FeCrAl steel. These materials are the material of choice for so-called interconnects in environmentally friendly solid oxide fuel cells (SOFCs). SOFCs combine high efficiency and fuel flexibility and is expected to be one of the technologies that will enable the transition towards a sustainable energy system, however the nature of the protective surface oxide layer, especially regarding the possible presence, nature, and role of hydrogen (H) in this layer, is not fully understood. This lack of understanding hampers the development of next generation materials for SOFCs.

How the work was done – The project was carried out by staff in my research group at the Department of Chemistry and Chemical Engineering at Chalmers, as well as by collaborating researchers at Sandvik Materials Technology (SMT). As a first step of the research, a series of samples, exposed to typical SOFC operating conditions, was prepared at Chalmers. These samples were then subjected to NR measurements at the Swedish Super ADAM beamline at the Institut Laue-Langevin (ILL) in Grenoble, France. A somewhat unexpected finding from this very first NR experiment was the observation of a large surface roughness, which we believe originate from the thermal growth of the protective oxide layer. To measure on samples with a lower surface roughness, which is normally needed for obtaining a high-quality NR pattern, special attention later in this project was directed to the preparation of more flat samples.

Results and expected impact – Figure 1 shows the NR data as measured on the sample exposed to SOFC condition (green), as well as on a substrate (black), *i.e.* an unexposed sample. Analysis of the NR data suggests that the exposure leads to an increase of the surface roughness from ≈1 nm (on the surface of the substrate) to ≈5 nm. Furthermore, the analysis indicates that the ≈5 nm roughness is mainly at the oxide/air interface, meaning that the low roughness at the substrate/oxide interface is virtually unaltered under exposure. This is an important new result that provides insight into the oxidation mechanism of the material and that encourages further NR studies, such as on a systematic series of films varying in exposure time.

Nonetheless, it should be noted that the increase in surface roughness causes a damping of the oscillations of the NR pattern, see e.g. the calculated NR curve in Figure 1. This effect makes the extraction of the chemical composition and quantification of H in the film very difficult. This encourages the use of alternative sample preparation techniques, such as sputtering, to prepare atomically flat samples, which is planned for this future. Crucially, we recognize the unique potential of further NR experiments on these kind of samples and, for this reason, we are committed to continue this track outside the scope of this project.

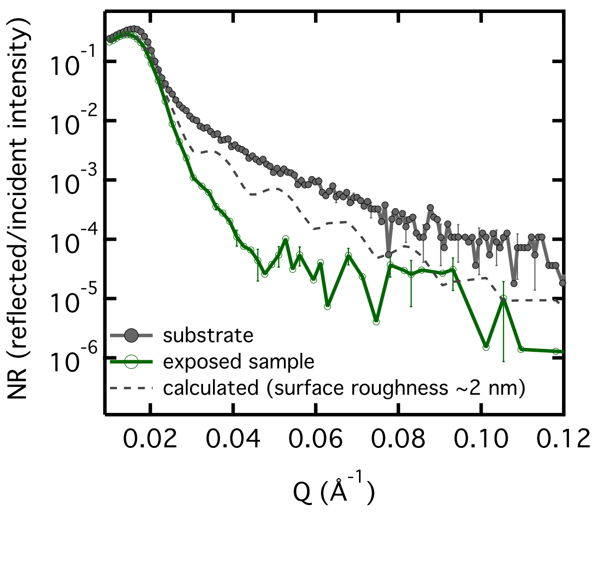

Figure 1. NR curves as measured on the substrate (black) and an exposed sample (green). A calculated curve for the case of a sample with low roughness (gray, dashed) is also shown