INDUSTRIAL PILOT PROJECT

Understanding of solar cell sensitization process using synchrotron based XAS and XPS

THE INDUSTRIAL CHALLENGE

EXEGER is a Stockholm-based solar cell company specialized in producing third generation dye sensitized solar cells (DSSCs). Efficient sensitization with high reproducibility for the technology developed by EXEGER is one key parameter in manufacturing. This process benefit from understanding of how the sensitization process affects the obtained surface structure at an atomic level.

WHY USING A LARGE SCALE FACILITY

Synchrotron sources like MAX IV generate ultra-high brilliance photons and enable measurement at ambient pressure. Using X-ray Photoelectron Spectroscopy (XPS) at pressures approaching the vapor pressure of solvents used in DSSC allows non-destructive investigation of molecular layers. Such studies can capture the fundamental processes occurring at surfaces during sensitization. Such detailed knowledge is complementary to another synchrotron technique, namely X-ray Absorption (XAS) which helps identifying parameters that must be optimized for further developing DSSCs sensitization procedure.

HOW THE WORK WAS DONE

The work was divided into two specific beam times at MAX IV: (1) XPS at the HIPPIE beamline, and (2) XAS at the BALDER beamline. We investigated metal-organic dyes having a ruthenium metal-centre. We used XPS to investigate effects on the metal-organic dye molecular layer after exposure to electrolyte solution, see Figure. Specifically, we compared the S2p core-level signals for dry samples and samples exposed to the electrolyte. XAS at the ruthenium K-edge was measured on powders of three known standard dyes pressed into 3 mm diameter pellets and compared to the DSSC dyes. Measurements were also done on sensitized thin films to follow the sensitization process. Spectroscopic signals were quantified, among other things, by following the time evolution.

THE RESULTS AND EXPECTED IMPACT

Data analysis of samples with a metal-organic dyes show (i) high similarity of films from different dye batches, (ii) no significant asymmetric distortions within the metal-centre environment, and (iii) indication on sensitization time needed for surface saturation. In studies on solvent effects, we observed changes in binding configuration when exposed to the electrolyte. This was interpreted as a tilt of the dye due to the effects from electrolyte molecules. A deeper analysis showed that the EXEGER dyes suffered from X-ray damage when measured in the presence of a liquid. This, in turn, show the importance of further developing measurement protocols for understanding of dye saturation.

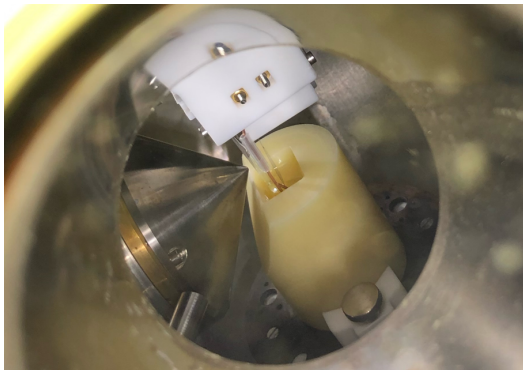

Figure. The measurement configuration for XPS at the HIPPIE beamline. The glass substrate with the sensitized sample is dipped into the electrolyte solution. The focus of the X-ray at MAX IV allows the cone of the analyser to be close to the sample. This, in turn, allows for measurements at high pressure.

"To use analysis equipment compatible with industrial samples is key in developing manufacturing techniques"
/Sven Södergren, EXEGER

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