



MATERIALS AND PROCESS ANALYSIS

IN-SITU AND OPERANDO STRUCTURAL INVESTIGATIONS OF ELECTROCHEMICAL SYSTEMS

Dr. Björn Matthey, Dr. Christian Heubner, M. Sc. Christoph Lämmel, Dr. Michael Schneider, Dr. Mathias Herrmann

Electrochemical processes and systems are considered key technologies for sustainable production and energy sectors. This includes innovative coating processes as well as devices for electrochemical energy storage and conversion. Knowledge-based development and optimization of such systems requires a fundamental understanding of the ongoing reactions and potential degradation processes. In-situ and operando structural investigations by means of X-ray diffraction (XRD) allow a particularly detailed clarification of reaction mechanisms and resulting correlations between processes, structures and properties, based on complementary electrochemical and structural information. Fraunhofer IKTS develops customized electrochemical cell designs (Figure 1) for complementary in-situ and operando structural investigations (Figure 2).

Functional coatings

The most relevant properties of functional coatings are mainly determined by their microstructure. At Fraunhofer IKTS, in-situ XRD measurements are carried out to clarify the microstructural development during the fabrication of functional coatings. Corresponding results allow to determine and develop phase composition and microstructural parameters, such as crystallite size and microstrains, during deposition, depending on the electrochemical manufacturing conditions. Accordingly, process-structure-property correlations can be derived in order to optimize processes in a targeted way.

Energy storage systems

The development of innovative systems for electrochemical energy storage and conversion is accompanied by complementary operando structural investigations by means of XRD and Raman spectroscopy. The measurements enable comprehensive insights into mechanisms and the reversibility of structural and compositional modifications during operation. Using knowledge gained, it is possible to develop novel lithium- and sodium-ion batteries as well as hybrid systems with a focus on enhanced power capability and improved long-term stability.

Services offered

- Development and validation of electrochemical cell designs for in-situ and operando structural investigations by means of XRD and Raman spectroscopy
- Phases and structural parameters
- Analysis of process-structure-property correlations



- 1 *Electrochemical operando XRD cell developed at Fraunhofer IKTS.*
- 2 *Phase analysis using X-ray diffraction (XRD) during electrochemical Li/Na substitution in LiCoO₂.*