LEHRSTUHL
LEE Energieverfahrenstechnik & Energiesysteme

UNIVERSITÄT DUISBURG ESSEN
Offen im Denken

Master-/ Bachelorarbeit

„Elementary Kinetics, Surface Dynamics, and Reversible Operation of a Solid Oxide Cell in Python/Cantera“

Allgemeines:

A previous work successfully developed a numerical single-cell model based on elementary electrochemical kinetics in Python/Cantera, capable of replicating polarization (I-V) curves for two experimental datasets. To move beyond this proof of concept, the model needs to be validated across a broader array of experimental data. Additionally, expanding the scope to Reversible Solid Oxide Cells (rSOC) by incorporating electrolysis mode (SOEC) is essential for evaluating grid-flexible energy storage applications. With the model extended and verified, a closer look will be given to the elementary kinetics, the surface coverages and the rate-determining step.

Aufgabenstellung:

- Assess the state of the Art of SOC modeling, with a focus on an elementary kinetics approach
- Validate the elementary kinetics model against a wider set of published experimental I-V curves across varying temperatures, pressures, and steam concentrations.
- Perform a deeper kinetic analysis to identify the rate-limiting steps at the triple-phase boundaries and examine how these steps shift under different operating conditions.
- Map the steady-state surface coverages of intermediate species across varying potentials to assess active site availability
- Extend the model framework from power generation mode (SOFC) to electrolysis mode (SOEC), evaluating model consistency and kinetics under reverse current loads.

Bei Interesse wenden Sie sich per Mail (inkl. Lebenslauf und Notenspiegel) an:

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