Basic research predicting the behaviour of cathodes and electrolytes in SOFCs

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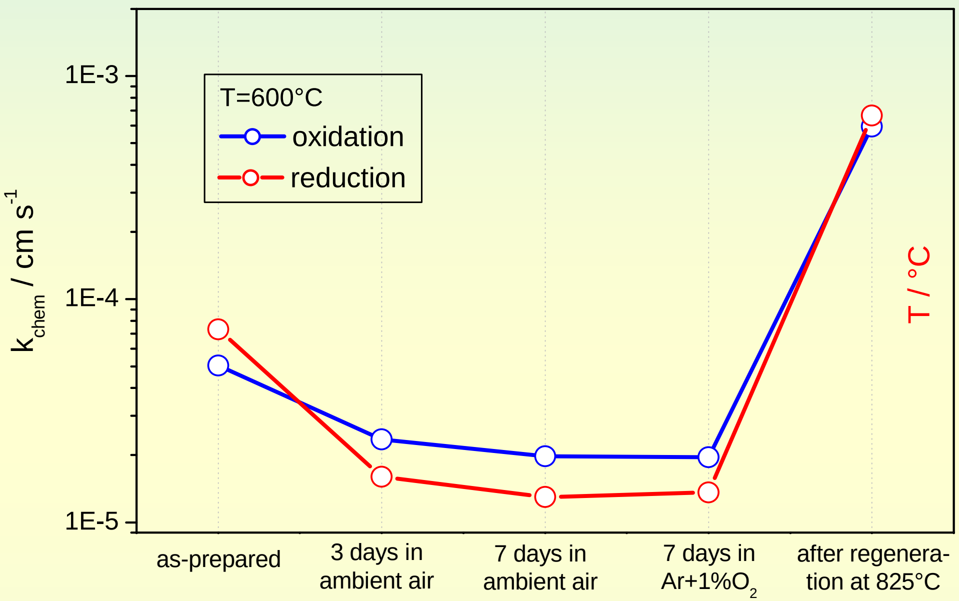
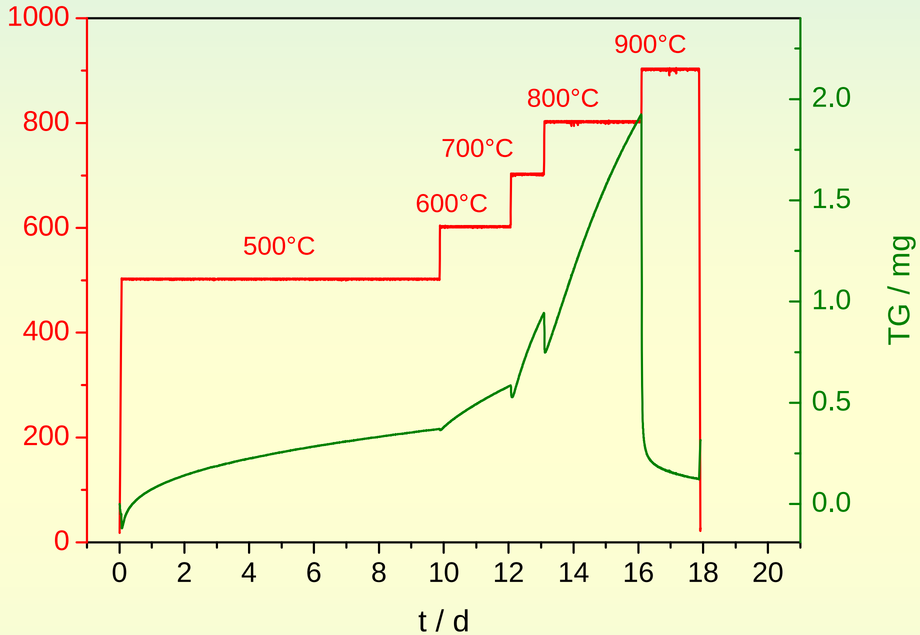
Predictive basic research - also with respect to cell degradation

Cathodes

- Search for new electrode materials with excellent oxygen exchange properties also at reduced temperatures
- Oxygen exchange properties (k_{chem}, D_{chem}) e.g. of cathodes under *real conditions* (CO_2, H_2O, ...) in order to predict the long-time stability
- Modelling of electrode performance with optimized microstructure from fundamental parameters (k_{chem}, D_{chem}, ...)
- Surface (XPS, SIMS, TEM ...) and interface analysis (SEM, TEM...) in order to predict the long-time stability

Example: Insufficient stability of BSCF vs. CO_2





Decrease of k_{chem} of BSCF at 600°C due to CO_2-containing atmospheres

Significant carbonate formation of BSCF in 5% CO_2, regeneration at T>800°C

E. Bucher, A. Egger, G.B. Caraman, W. Sitte, J. Electrochem. Soc. 155 (2008) B1218.

Example: D_{chem} and k_{chem} as input parameters for modelling the ASR of a SOFC-Cathode

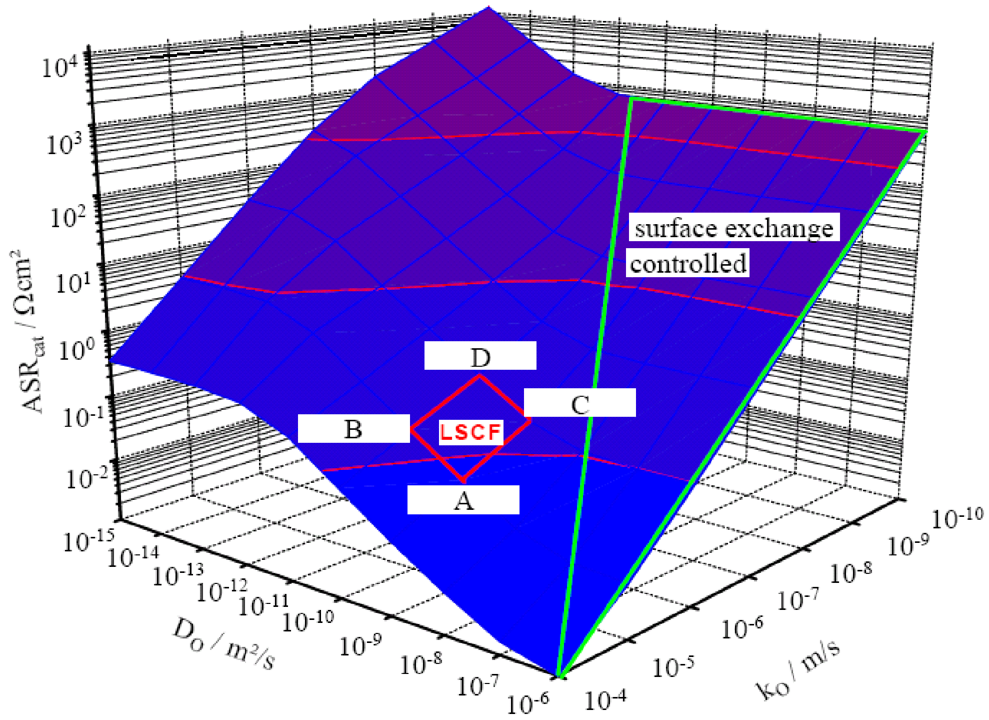


Figure 3. The area specific cathode resistance ASR_{cat} at 800 °C averaged from ~15 simulations is depicted dependent on bulk diffusion D_O and surface exchange coefficient k_O. A 7x7x40 model was used with a porosity of 40 %, a cathode thickness l_{cat} of 30 µm and a cube length l_{cu} of 750 nm.
(T = 800 °C, σ_{El} = 4.72 S/m, η_{Model} = 0.1 V, ASR_{CT} = 0.1 mΩcm², p = 1 bar, p_{GC} = 0.21 bar, $p_{CE} = 10^{-23}$ bar)

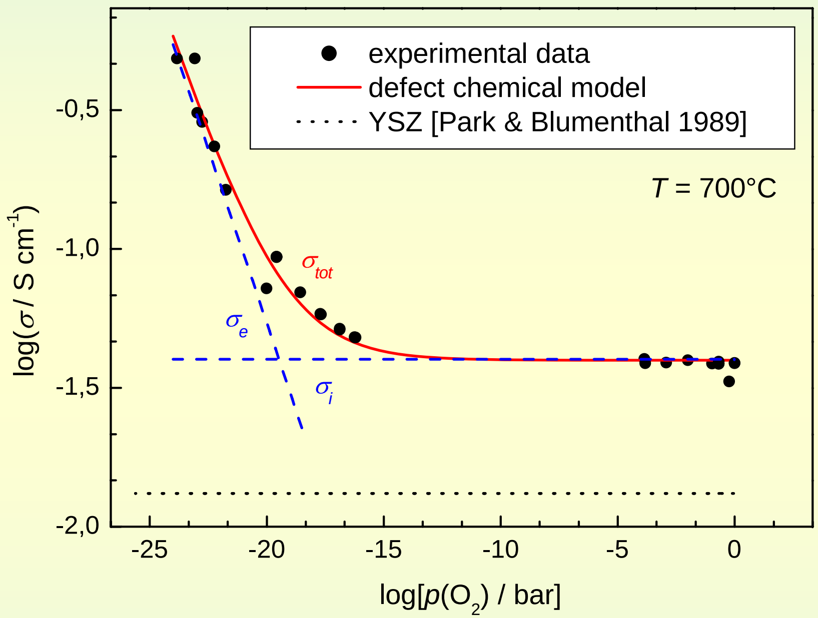
B. Rüger et. al., SOFC-X, Nara, Japan, 2007.

Predictive basic research - electrolytes

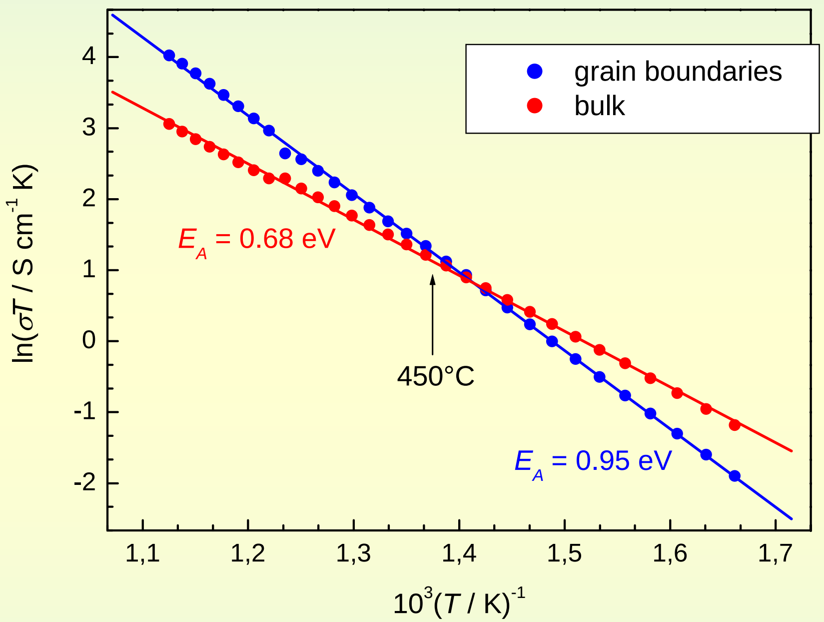
- Search for new electrolytes with high ionic conductivities also at reduced temperatures
- pO_2- and temperature dependence of bulk and grain boundary conductivities (electrolytic domain, electronic conductivity)
- long-time stability (phase stability, chemical stability against electrodes and partial reduction, …)
- Surface and interface analysis in order to predict the long-time stability

Example: $Ce_{0.90}Gd_{0.10}O_{1.95}$

pO_2-dependence



Arrhenius-plot

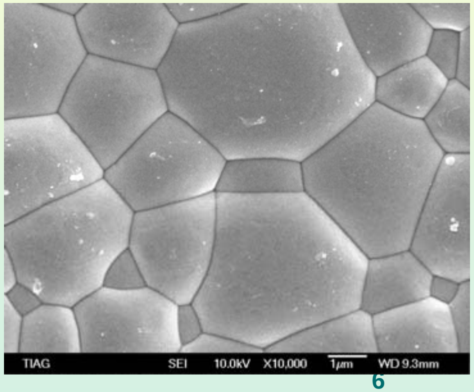


Defect chemistry

$$\sigma_{tot} = \sigma_e + \sigma_i$$

$$\sigma_e \propto p(\mathrm{O}_2)^{-1/4} \text{ and } \sigma_i = const$$

Microstructure:
d_g = 3 – 5 µm



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