**Tuesday, Part A / Talk No. 2**

## Elementary kinetic modeling and experimental validation of CO electrooxidation on Ni/YSZ pattern anode

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In practical solid oxide fuel cell systems nickel and yttria-stabilized zirconia (Ni/YSZ) composites are frequently used as anodes. The elucidation of the microscopic details of the electrochemical reaction mechanism requires elementary kinetic numerical simulations along with electrochemical characterization experiments performed with geometrically well-defined model anode structures [1].
In the present work, the results of a comprehensive modeling and experimental study of electrochemical CO oxidation on well-defined Ni/YSZ patterned model anodes are presented. A computational model representing the coupled behavior of heterogeneous chemistry and electrochemistry in terms of elementary reactions was developed (Fig. 1 left), which allows for a quantitative description of the complete experimental data set, which covers a wide range of $CO/CO_2$ gas compositions ($4.0 \cdot 10^2$ Pa $\leq p_{CO} \leq 5.1 \cdot 10^4$ Pa and $9.5 \cdot 10^2$ Pa $\leq p_{CO2} \leq 9.2 \cdot 10^4$ Pa and operating temperatures (973 K $\leq T \leq$ 1073 K) (Fig. 1 right).

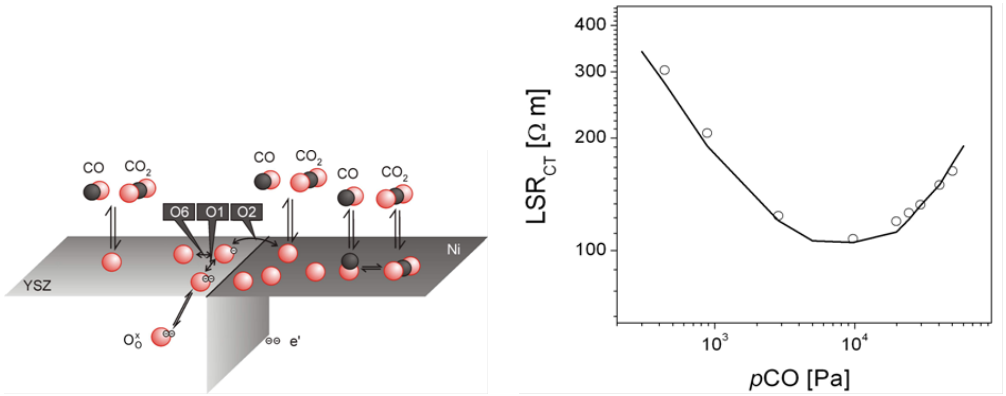


Figure 1: left – Schematic illustration of the reaction mechanism and the different charge-transfer pathways taking place at the three-phase boundary of Ni, YSZ and gas phase; right – Comparison between experimental (open symbols) and simulated (lines) line-specific resistance (LSRCT) of a Ni/YSZ pattern anode as a function of CO partial pressure for a constant $CO_2$ partial pressures of $2.0 \cdot 10^4$ Pa at $T = 1073$ K.

### References

[1] Bessler, Wolfgang G.; Vogler, Marcel; Störmer, Heike; Gerthsen, Dagmar; Utz, Annika; Weber, André; Ivers-Tiffée, Ellen, PCCP, 12 (2010), pp 13888-13903.