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/CO2 gas compositions (4.0 · 10^2 Pa ≤ pCO ≤ 5.1 · 10^4 Pa and 9.5 · 10^2 Pa ≤ pCO2 ≤ 9.2 · 10^4 Pa and operating temperatures (973 K ≤ T ≤ 1073K) (Fig. 1 right).

References