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# Atmosphere, temperature and pressure dependent segregation of bulk impurities in yttria-stabilized zirconia

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Control and characterization of extremely clean surfaces are important to gain fundamental understanding of processes on surfaces. All surfaces exposed to atmospheric conditions are covered with impurity adsorbates. These adsorbates are usually mainly water and organic molecules which lower the surface free energy of the external surface of the material. In devices operated at elevated temperatures (600 – 1100 ºC), such as solid oxide fuel cells (SOFCs), segregation of bulk impurities from component materials can also be observed [1].

Bulk impurities present in yttria-stabilized zirconia (YSZ), typically used as electrolyte in SOFCs, such as silicon dioxide (silica), segregates to the anode-electrolyte interface at operating conditions of SOFCs. Impurity segregation and the formation of an impurity phase on YSZ have previously been shown to increase the polarization resistance of an anode-electrolyte SOFC model system [2].
Here we report on an in-situ ultra high vacuum (UHV) study of impurity segregation in YSZ single crystals.

YSZ single crystals were heated in an UHV chamber in the temperature range 750 – 1400 °C. Oxygen and water vapor atmospheres in the pressure range from UHV to 1 bar were introduced while the single crystals were annealed in the chamber. The single crystals were after treatment transported in-situ to an analysis chamber where X-ray photoelectron spectroscopy (XPS) measurements were performed. This setup allowed for investigation of the surface composition of YSZ without exposure to air.

All single crystals annealed in a furnace (ex-situ) at atmospheric conditions (1100 ºC, 1 bar) showed the formation of a silicon monolayer on the surface as characterized by angle-resolved XPS. Annealing in UHV at a range of elevated temperatures indicated a strong atmosphere dependency of silica segregation. Experiments with both low (< 1E-5 mbar) and high (> 1 mbar) pressures of water vapor and oxygen gas supported atmosphere dependence of silica segregation in YSZ. Furthermore, the experiments with water vapor and oxygen gas also revealed a temperature and pressure dependent silica segregation mechanism in YSZ.

The above findings indicate a strong dependence on atmosphere, pressure and temperature of silicon segregation in single crystal YSZ. Knowledge of the segregation process in YSZ allows for optimized cleaning cycles with the aim of producing extremely clean YSZ for electrochemical tests.

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