

Nickel Migration in SOFCs Anode due to Phosphine Induced Degradation: A Computational Study

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A major hindrance for utilization of coal gas in Solid Oxide Fuel Cells (SOFC) is poisoning of SOFC anode materials by the impurities in coal. One such impurity, phosphine is known to cause catastrophic failure of SOFC anode even at concentrations below 10 ppm. A significant phenomenon observed in SOFC anodes, made of Ni-YSZ cermets, exposed to phosphine is migration of the nickel from porous matrix to the surface, which is believed to be one of the reasons for performance degradation. The mechanism responsible for the experimentally observed Ni migration is not well understood. In this study, a possible mechanism is proposed for Ni migration in SOFCs and its aptness for predicting Ni migration is verified using numerical modeling. It is postulated that the gradients in volumetric concentration of nickel inside the anode, set up due to lower porosity in the active region compared to the support layer, could potentially cause Ni diffusion. Upon phosphine exposure, the Ni on the surface layer is the first to react and form secondary phases causing the Ni concentration to decrease further at the surface. This will drive the diffusion of Ni from the bulk of the porous anode to the surface. The diffusion of Ni is further accelerated by the secondary phase formation since the diffusivity of Ni in Ni-P compounds is much higher than that in the YSZ. The melting point for some secondary phases is close to the cell operating temperature causing them to soften and thus be more conducive for Ni migration. A transport model for nickel migration is formulated based on these postulations and it is integrated into an existing one dimensional code for predicting SOFC anode degradation due to fuel impurities. Simulations show that the proposed mechanism of Ni diffusion driven by secondary phase formation can emulate the experimentally observed accumulation of Ni and Ni-P compounds on the SOFC anode surface when exposed to phosphine.