Rational Design of Sulfur-Tolerant Anode Materials for Solid Oxide Fuel Cells

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Solid oxide fuel cells (SOFC) offer great potential for significantly higher efficiency for power generation with reduced emission of pollutants. Apart from pure hydrogen, SOFC also have the potential to directly utilize hydrocarbon fuels, which are readily available and easier to transport and store. However, the state-of-the-art nickel-yttria stabilized zirconia (Ni-YSZ) cermet anode for SOFCs is susceptible to poisoning by ppm-level sulfur contaminants typically found in most hydrocarbon fuels, leading to severe performance loss or even cell failure. This problem calls for the development of new sulfur-tolerant anode materials for SOFC with high electrochemical activity.

In light of such a research need and the "trial-and-error" nature of previous studies in this area, this presentation aims at providing some insights into the rational design of sulfur-tolerant anode materials for SOFC from two independent aspects. The first one focuses on using thermochemical analysis and associated experiments as a powerful tool for the designing and quick screening of sulfur-tolerant anode materials for SOFC. It will be demonstrated by an interesting example in the understanding and prediction of the chemical stability of $LaVO_3$-$SrVO_3$-$LaTiO_3$-$SrTiO_3$ series materials against hydrogen sulfide (H_2S) contaminant. The second aspect is on applying insights about the fundamental sulfur poisoning mechanism for conventional Ni-YSZ cermet anode to guide the design of new sulfur-tolerant anode materials. From this perspective, different sulfur-tolerant anode materials proposed will be analyzed, and the effectiveness of such an approach is illustrated through the discovery of a new class of sulfur-tolerant anodes with the YSZ oxygen-ion conductor in the conventional Ni-YSZ cermet anode replaced by proton-conducting oxides such as $Ba(Zr_{0.1}Ce_{0.7}Y_{0.2-x}Yb_x)O_{3-\delta}$ (BZCYYb) while keeping Ni as the electrical conductor and catalyst. The Ni-BZCYYb cermet anode demonstrates a uniqueness of improved sulfur-tolerance by more than two orders of magnitude (from ~0.05 to > ~20ppm) while maintaining high electrochemical activity comparable to the Ni-YSZ cermet anode. The presentation will conclude with a discussion of the remaining challenges and future research directions in this field.