Operando oxidation and reduction neutron scattering studies on pristine and Pt-coated ceria nanorods

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Ceria is widely used as a three-way catalyst support (TWC) for the conversion of automotive emissions due to its excellent redox properties and high oxygen storage capacity (OSC). It has been broadly reported that OSC can be drastically improved by increasing the concentration of oxygen defects and that the redox properties of ceria are controlled by the type, size, distribution, and location (surface or bulk) of the oxygen vacancies. Recently, a partially reduced Ce3O5+x defect phase was discovered on the surface of ceria nanorods, which is distinct from the bulk Frenkel-type defect structure. The higher OSC performance of ceria nanorods relative to other morphologies (such as nanocubes) was attributed to the presence of a higher concentration of these surface defects.

Platinum group metals have been shown to strongly interact with ceria under redox conditions, further improving its catalytic properties. In this work, we elucidate the effects of Pt loading on the surface and bulk defects of ceria nanorods, through an in situ neutron scattering study of as prepared vs 1% Pt-coated ceria nanorods, under redox flow. Bragg diffraction results indicate that the bulk structure of both as prepared and 1% Pt-coated ceria nanorods can be indexed to a classic Fluorite structure. Interestingly, pair distribution function analysis (PDF), in accordance with Bragg results, indicate that the Pt-coated rods have a larger lattice parameter and crystallite domain size than the as prepared rods. This suggests that the Pt-coated rods contain a higher concentration of Ce3+ and are more easily reducible than the as prepared rods. Further PDF results reveal that the Pt-coated rods contain a secondary surface defect phase, which is lacking in the as-prepared rods. These structural differences in the as prepared and Pt-coated rods explain the superior catalytic performance of the Pt-coated rods. Unlike many studies in scientific literature, the as prepared and Pt-coated nanorods used in this study more closely resemble real catalytic converters, which are pre-conditioned at high temperatures in humid oxidizing conditions. Thus, the results from this study provide insights into the structure of ceria nanorod based catalysts under real operating conditions, which can aid in the design and optimization of future catalytic materials.