NAPLES, ITALY 23-27 JUNE
DSL2025 NAPLES
21st International Conference on Diffusion in Solids and Liquids

ABSTRACT

Local Structure and Dynamics of Protons, Holes and Hydride Ions in Perovskite-Type Oxides

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Perovskite-type oxides such as $BaZrO_3$ have attracted much attention as host materials for ionic conductors. In addition to oxide ions, protons and hydride ions are highly mobile in perovskite-type oxides. In general, acceptor doping is effective for introducing such mobile species. Meanwhile, the defect equilibrium compensating for the effective negative charge of the acceptor is complicated and exhibits a trade-off relationship. Defect equilibrium also includes electronic compensation, that is, electron holes. In other words, controlling the amount and diffusivity of the mobile species is challenging. This study provides a comprehensive understanding of defect compensation in Sc-doped $BaZrO_3$ (BZS) by protons, electron holes, and hydride ions. Fully oxidized BZS with only electronic holes was prepared using a high-pressure apparatus under 6 GPa at 700 °C with a $KClO_4$ oxidant. The hole concentration was comparable to that of the proton concentration for hydrated samples. The local structures and dynamics of BZSs with different mobile species were analyzed using temperature-variable solid-state NMR. In addition to protons and electron holes, hydride ions were successfully introduced into BZS via a topochemical reaction. Their local structures and dynamics are discussed by combining NMR and DFT calculations.