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A comparative proton conductivity study on Yb-doped BaZrO₃ perovskite at intermediate temperatures under wet N₂ environment

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Abstract: Conventional solid state reaction route was used for the synthesis of oxygen deficient BaZr_{1-x}Yb_xO_{3-δ} ($x = 0.05, 0.10, 0.15, 0.20$) oxide. Rietveld refinement of x -ray diffraction data confirmed the formation of mono-phasic cubic perovskite structure with space group $Pm\bar{3}m$. The microstructure coupled with EDX analysis of the sintered ceramics reveals the formation of sub-micron sized grains, with no detection of impurity elements. Thermogravimetric analysis of the pre-hydrated sample shows a significant mass loss suggesting complete filling of oxygen vacancies by protonic defects. Impedance spectroscopy performed under wet N₂ environment show highest proton conductivity for the composition with $x=0.20$. The total conductivity at 600°C significantly increased from the order of 10^{-5} Scm⁻¹ for $x=0.05$ to 10^{-3} Scm⁻¹ for $x=0.20$ composition. The activation energy calculated from the Arrhenius dependence of total conductivity decreased with an increase in trivalent Yb³⁺ concentration, since the number of charge carriers in the form of protonic defects increases.

Keywords: Oxygen vacancies, Perovskite, Proton conductivity, Protonic defects

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