

Title: The dopant effect of proton trapping in barium zirconate

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Abstract: The electrical conductivity of BaZrO₃ doped with Gd, Y, or Lu has been studied by the two-probe ac technique in the temperature range 307-1073K. The chemical diffusion coefficients of proton/deuteron diffusion pair (isotope diffusion coefficient) were determined by the relaxation time of the ohmic resistance change upon the substitution of the atmosphere from H₂O to D₂O. Moreover, the diffusion coefficient of proton was determined using the conductivity in combination with the concentration of proton by thermogravimetry. The proton diffusivity curves downward in an Arrhenius plot. At high temperatures the slope corresponds to an activation energy of 18 kJ/mol for all samples, whereas at low temperatures it corresponds to a greatly increased activation energy of 45 kJ/mol for BaZrO₃ doped with Y or Lu. The activation energy of BaZrO₃ doped with Gd was 58 kJ/mol. Evaluation of the curvature in the context of a trapping model implies a proton binding energy of 27 kJ/mol for Y or Lu and 40 kJ/mol for Gd.