

CRYSTAL STRUCTURE, OXYGEN NONSTOICHIOMETRY, HYDRATION AND CONDUCTIVITY BaZr_{1-x}M_xO_{3-d} (M=Pr, Nd, Y, Co)

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Partially substituted perovskite-like barium zirconates with general formula BaZr_{1-x}M_xO_{3-d} possess oxygen-ion and proton conductivity and, therefore, may be promising as electrolytes for intermediate temperature solid oxide fuel cells. The aim of this work was to study the crystal structure, thermal and chemical expansion, water uptake, oxygen nonstoichiometry, total conductivity and Seebeck coefficient of zirconates BaZr_{1-x}M_xO_{3-d} (M=Pr, Nd, Y, Co) in the atmospheres with different levels of humidity ($\log(p_{H_2O}/atm.) = -1.75; -2.5; -3.5$) as a function of oxygen partial pressure ($\log(p_{O_2}/atm) = -20 - -0.67$) and temperature ($T = 25 - 1050$ °C).

Synthesis of the samples was carried out by glycerol-nitrate method. The phase composition of the as-prepared powders was analyzed by the X-ray diffraction (XRD). Room temperature and high temperature XRD studies were carried out using Shimadzu XRD-7000 diffractometer equipped with high temperature chamber HTK 16N (Anton Paar GmbH). Thermal and chemical expansion was also measured using DIL 402 C dilatometer (Netzsch GmbH). Oxygen nonstoichiometry was studied by solid state coulometric titration and thermogravimetry. Electrical conductivity and Seebeck coefficient were measured simultaneously in the same setup.

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