SYNTHESIS, CRYSTAL STRUCURE AND TOTAL CONDUCTIVITY OF $La_{2-x}Ba_xNiO_{4\pm\delta}$

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The Ruddlesden-Popper-type oxides $La_{2-x}Ba_xNiO_{4\pm\delta}$ are considered to be prospective candidates to be used as cathode materials in Solid Oxide Fuel Cells (SOFCs) due to their relatively high mixed ionic and electronic conductivity (MIEC) [1-3]. The replacement of La^{3+} by Ba^{2+} causes extensive changes to the crystal structure, electronic transport behavior, and oxygen diffusivity [1].

In the current study the $La_{2-x}Ba_xNiO_{4\pm\delta}$ samples were prepared using a citrate-nitrate method followed by solid-state reaction at high temperature (1000-1100 ºC). Phase purity was studied by using X-ray diffraction (XRD).

Phase identification analysis reveals that the $La_{2-x}Ba_xNiO_{4\pm\delta}$ samples with x=0.2, 0.6, 0.8, 0.9 1.0 and 1.2 have the tetragonal K_2NiF_4-type structure (space group I4/mmm), whereas for x = 1.4 the formation of secondary phases such as $BaNiO_3$ or $La_6Ba_6Ni_4O_{18}$ was observed.

The temperature dependences of total conductivity and the Seebeck coefficient for $La_{2-x}Ba_xNiO_{4\pm\delta}$ (x = 0.2, 0.6) were measured in the range of 25-950 °C. The $La_{1.4}Ba_{0.6}NiO_{4\pm\delta}$ shows the highest electrical conductivity of 40.9 S/cm at 950 °C in air.

Electrical conductivity measurements confirm that charge transport follows a small polaron hopping mechanism, with enhanced conductivity at moderate temperatures and doping levels (x = 0.2–0.6) due to increased Ni^{3+} concentration and electron hole mobility with temperature. At high temperatures excessive oxygen vacancies cause a decrease in Ni^{3+} concentration reducing total conductivity.

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