MODELLING AND OPTIMIZATION IN La_2NiO_4-BASED MEMBRANES

Naumovich E.[1], Shaula A.[2], Viskup A.[3], Pankov V.[3], Kharton V.[1]

[1] *Ceramics and Glass Eng. Department, University of Aveiro, Aveiro, Portugal*
[2] *Department of Mechanical Engineering, ICEMS, University of Coimbra, Coimbra, Portugal*
[3] *Research Institute For Physical Chemical Problems, Belarus State University, Minsk, Belarus*

Mixed conductors based on K_2NiF_4-type lanthanum nickelate, $La_2NiO_{4+\delta}$, are of great interest as parent materials for the solid oxide fuel cell cathodes and ceramic membranes for oxygen separation and partial oxidation of hydrocarbons. Key advantages of La_2NiO_4-based compositions include substantial oxygen-ionic and *p*-type electronic conductivities, moderate thermal and chemical expansion, and high electrocatalytic activity under oxidizing conditions. The oxygen transport through dense nickelate ceramics is essentially limited by kinetics of electrochemical processes at the surface, which prevents bulk reduction and enables stable operation under large oxygen chemical potential gradients at the temperatures below 1173K.

This work is focused on the analysis of steady-state oxygen permeation through $La_2NiO_{4+\delta}$ membranes with different architecture. The gas-tight membranes with and without additional porous layers were prepared via the glycine-nitrate synthesis and tape-casting, followed by sintering; the characterization was performed X-ray diffraction, scanning electron microscopy combined with energy-dispersive spectroscopy, thermogravimetry, dilatometry, differential scanning calorimetry, and measurements of total conductivity and steady-state oxygen permeation fluxes in a wide range of temperature and oxygen partial pressure. The data on equilibrium oxygen nonstoichiometry, conductivity and oxygen permeability were used to develop a theoretical approach for the description of the bulk ambipolar diffusion and interfacial oxygen transfer through the membrane/gas boundaries. The model was validated employing experimental data on the oxygen permeability of $La_2NiO_{4+\delta}$ membranes with different thickness, architecture of tape-casted layers and ceramic microstructure.