Description for the general public

Possibility of usage a particular material in a specific technical application depends on whether it meets many, usually very strict, criteria concerning its physical and chemical properties. In most of the cases it is not possible to develop an ideal material that perfectly meets all the requirements. In practice, choice of safe and inexpensive materials that can provide long-term operation is preferred, even if such compounds exhibit worse other parameters related to the application. An alternative approach is also possible, using composite materials, in which the two (or more) of the components interact synergistically, in a way to maximally meet the requirements for the material-related properties (a good example in this regard is a simple case of the reinforced concrete).

In many electrochemical applications (such as in galvanic or electrolysis cells, and in the case of membranes) electric conduction, realized through an electronic component (motion of electrons) and ionic component (movement of various kinds of ions) is a key parameter in determining the possibility of usage of the particular compound in practice. Such a mixed ionic-electronic conductivity is also of interest to many researchers, due to the fact that it is dependent on a number of factors related to the chemical composition of the material and its internal structure (the type and arrangement of atoms), and the microstructure (i.e. size, shape and morphology of the grains of the material).

Scientific aim of the project focuses on development of ceramic membranes exhibiting high, mixed ionic-electronic conductivity. It will be achieved using advanced computations and experimental techniques, which will allow to select the best chemical composition in a group of complicated, layered oxides with $(Ln_{2-x}A'_x)_{1-y}Ni_{1-z}B'_zO_{4\pm\delta}$ (Ln - selected lanthanides; A' - Sr, Ba; B' - selected 3d metals, e.g. Cu; In, Ga) formula. Also, it will be realized through modification of the grain surface of the initial materials by formation of a functional layer of $A_{n+1}B_nO_{3n+1}$ oxide ($n > 1$, e.g. $Ln_3Ni_2O_7$), with suitably chosen chemical composition. Scientific interest in $(Ln_{2-x}A'_x)_{1-y}Ni_{1-z}B'_zO_{4\pm\delta}$ oxides stems from their good chemical stability, moderate thermal expansion and high ionic-electronic conductivity. These compounds meet many of the criteria required for manufacturing of good membranes. Their main disadvantage is, however, the nature of conduction of ions and electrons, which is a two-dimensional in space. Presented in the proposal is a new idea, which corresponds to the formation of the composite membrane, in which the base material has a very high ionic-electronic conductivity in two spatial directions, and the outer layer (modifying the grain boundaries) allows for an easy transfer of electric charges (ions and electrons) between the grains.

Project's methodology (i.e. a scientific way of achieving the project's objectives) consists of carefully planned research activities, including advanced numerical computations and state-of-the-art experimental techniques. The methodology concerns: computer calculations of the structural features of materials from $(Ln_{2-x}A'_x)_{1-y}Ni_{1-z}B'_zO_{4\pm\delta}$ group, advanced quantum mechanical calculations, synthesis of the materials via solid state and soft chemistry methods, crystal structure examination at room temperature, as well at high temperatures, complementary spectroscopy studies, measurements of mass changes of the samples as a function temperature, allowing determination of the oxygen content and its evolution on temperature, measurements of electrical conductivity (total, ionic and electronic components) and so called Seebeck coefficient as a function of temperature and oxygen content in the atmosphere, determination of surface exchange coefficient k and bulk diffusion coefficient D from relaxation-type measurements (these are very important parameters characterizing transport properties), measurements of thermal and chemical expansion, as well as chemical stability studies and determination of the oxygen permeation properties of the membranes as a function of temperature and membrane's thickness.

The proposed methodology is planned in a way to effectively utilize human and technical resources, with a significant role of numerical computations, which will allow to decrees number of samples needed for studies, only to the most promising and scientifically interesting ones. Successful accomplishment of the project's tasks shall have major impact on progress of solid state chemistry and physics in terms of understanding mechanism of ionic and electronic transport in dense mixed ionic-electronic conducting membranes. Overcoming the critical issues in the considered group of oxides will enable to obtain optimized compounds and microstructurally-modified sinters with enhanced useful properties. This, in turn, will be of great importance for further development of technology of ceramic membranes for partial oxidation of methane, gas separation, and generally, in clean and renewable power applications, and therefore societal impact of these studies cannot be underestimated.