Aims of the project

Project „Structural properties and ionic conduction mechanisms in doped ABO4 oxides" is concerned with structural and electrical properties of ceramics. Aim of this project are studies of the solid solutions of two different ceramics: LaNbO4 and LaSbO4 or LaNbO4 and LaAsO4.
Ceramics are polycrystalline materials, which can exhibit a different mechanical and electrical properties (e.g. ceramic material can be an insulator, semiconductor or a conductor). Materials studied in this project belong to the group of high temperature proton conductors. In these materials a charge carrier is an hydrogen ion, which differs them from typical conductors or semiconductors, where charge carriers are electrons or electron holes. Characteristic properties of high temperature proton conductor is that they do not have hydrogen in their nominal structure. Therefore hydrogen ion in these materials is a defect (a deviation from ideal crystal structure), which is called a protonic defect. Protonic defects are formed as a result of reaction of the material with its surroundings, e.g. reaction of the material with water vapour, which is described by following equation:
$H_2O(g)+ V_O^{**}+O_O^X=2(OH)_O^*$ (1)
From the equation (1) it is clear that water molecule reacts with oxygen ion and oxygen vacancy (empty space in a site normally occupied by oxygen ion) in the material structure and forms two OH groups on the oxygen sites with the relative plus charge (*- plus charge relative to an ideal crystal structure).
Proton conducting material can be called an electrolyte (when it conducts only protons) or mixed conductor (when it conducts protons and electrons in the same time). Depending on this property it can be used in different devices working with hydrogen, such as: gas sensors, hydrogen pumps and selective gas valves, fuel cells working with hydrogen as a fuel, hydrogen generating devices (steam electrolysers) or devices used to perform controlled reaction between selected compounds and hydrogen (e.g. hydrogenation/dehydrogenation of organics). Due to the fact that ceramics are not very reactive and they conduct protons only at elevated temperatures these materials can be used not only with hydrogen, but also with another hydrogen compounds, which require high temperature to react (e.g. direct fuel reforming in fuel cell).
Aim of this project is to find a new proton conducting materials, which structural and electrical properties can be "tailored" accordingly to the current needs by the change of material composition.

Basic research to be carried out in the project

In this project a series of basic research methods are planned. First of all material structure and microstructure will be measured by X-ray diffraction and scanning electron microscopy. Processes involving change of structure with the temperature will also be studied.
In the next stage of this project a thermal properties will be studied. Thermal expansion coefficient measurements, mass change with temperature, heat flux change with temperature and other studies will provide an information about reactions and processes inside the material. On this stage techniques such as dilatometry, thermogravimetry with mass spectroscopy and differential scanning calorimetry will be used. Main task of this stage is to determine the ongoing processes in the wide range of temperatures and information about defect concentration (such as oxygen vacancies and protonic defects).
During third stage an electrical properties will be studied. Conductivity in varying temperature, atmosphere (e.g. oxygen, air, hydrogen) and humidity conditions will be measured. Measuring conductivity as a function of temperature, oxygen partial pressure and water vapour partial pressure will help to determine conductivity mechanisms and dominating charge carriers. As a measuring technique an electrochemical impedance spectroscopy and 4-point DC conductivity measurement method will be used. On this stage an X-ray photoelectron spectroscopy will also be used. This technique, in fact, does not measure an electrical properties, but it provides information about oxidation states of elements in the material and therefore in will provide additional data about possible charge carriers existing in the material.
The last stage of the project will consist mostly on in-depth analysis of relations between different properties measured in the prior stages. The structural data combined with thermal and electrical properties will lead to determining the relation between defects and conduction mechanisms in the material. As a result a theoretical model will be proposed in order to connect relations between the defect chemistry and final material properties.

Reasons for choosing the research topic

This topic is important, because it fits in the trend of the search for new ion conducting materials. Such materials are in demand in the hydrogen-based technologies. Hydrogen technologies, which are considered as a branch of energy industry, are focused on the problem of transport, storage and conversion of hydrogen fuel into electric energy. Hydrogen technologies are considered to be an fundamental element of modern electrical grid, which will be effective and environmental friendly.