Instytut Fizyki Molekularnej PAN

Wpływ ciśnienia na mechanizm transportu elektrycznego w selenianach amonowych o różnych stechiometriach

ROZPRAWA DOKTORSKA

mgr inż. Łukasz Lindner

Promotor:
dr hab. Maria Zdanowska-Frączek, prof. IFM PAN

Poznań, 2017

Abstract

The doctoral dissertation is concerned with investigation of transport phenomena in selected proton conductors, that is ammonium selenates of different stoichiometries, such as $(NH_4)_3H(SeO_4)_2$ and $(NH_4)_4H_2(SeO_4)_3$, belonging to the class of crystalline solid acids. Superprotonic properties of this group of materials have attracted much interest due to their potential use as solid electrolytes in electrochemical devices, particularly in fuel cells.

The crystals were selected so that they could make model molecular systems for investigation of nonlinear effects in the process of charge transport and meet the criterion of having capacity above 10^{-2} S/cm.

The mechanisms of electric transport phenomenon, the kinetics of superionic transition and the role of NH_4^+ cations were analyzed. The main method of investigation was impedance spectroscopy under hydrostatic pressure. The results were supplemented and supported with the ^1H NMR measurements and computer simulations designed for one of the crystals studied and based on the Kinetic Monte Carlo method.

The results permitted to propose a mechanism of proton transport, pathways of charge transport and the role of NH_4^+ in the process of conduction. An interesting finding was the significance of geometry of hydrogen bonds involved in the charge transport pathway. Attempts were made to explain phenomena accompanying the transitions to superprotonic phases. The kinetics of transition of $(NH_4)_4H_2(SeO_4)_3$ crystal to the superionic phase at fixed thermodynamic conditions was studied assuming the Avrami model.