

Novel solid electrolytes for lithium-ion batteries: exploring the relationship between structure and electrical properties of LiTa_2PO_8 -based ceramics

Today, rechargeable lithium-ion batteries have become the most popular energy source for various applications: portable electronics, the automotive industry, and green energy storage systems. Despite its worldwide success, this technology still has its limitations. Therefore, continuous effort is being made by scientists in order to develop the next generation of lithium-ion cells, safer and more efficient than conventional ones. What can revolutionize lithium-ion technology is the replacement of liquid electrolytes by their solid counterparts. Liquid electrolytes are toxic and flammable. Therefore, they pose a risk in the event of damage or leakage. Solid electrolytes could, in principle, improve the safety and reliability of Li-ion cells as well as improve their parameters (operational voltage, energy density, cyclability) and enable their miniaturization. An intensive search for solid electrolytes is currently underway, and the progress that has been made in this field proves that this goal is achievable in the near future.

In this project, we propose systematic research on a new, ceramic lithium-ion conductor, lithium tantalum phosphate LiTa_2PO_8 (LTPO). Despite many advantages (e.g., good grain conductivity, stable crystal structure), its total electrical conductivity is still insufficient to compete with liquid electrolytes. It is worth mentioning that two factors are responsible for the total ionic conductivity of ceramic materials: the grain conductivity and the grain boundary one. So, the increase of these two components of conductivity should improve the total conductivity and enable the construction of prototype cells with LTPO-based ceramic as solid electrolyte.

Based on our previous research and on literature reports, we claim that the electrical properties of LTPO can be significantly improved in two ways. Firstly - by using appropriate dopants, that is, by substituting some atoms in the crystal lattice with others. The presence of appropriate dopants is supposed to improve the mechanism of grain conductivity. Secondly – by appropriate sintering with the use of Upgraded-Field Assisted Sintering Technology (U-FAST) – thanks to it, one can modify the microstructure of ceramics (porosity) and the properties of grain boundary region. That should lead to the improvement of the grain boundary conductivity.

The experimental work includes the synthesis of several families of LTPO-based ceramics and the study of their properties by means of a set of experimental methods, including: X-ray diffraction, Raman spectroscopy, nuclear magnetic resonance spectroscopy, thermomechanical and thermogravimetric analysis, electron microscopy, impedance spectroscopy, transference numbers measurement. It is worth emphasizing that the materials under study have not been described in the literature before.

As a result of our research, we intend to identify and describe the relationship between the crystal structure, microstructure and electrical properties of new, previously unexplored LTPO-based ceramics. We will come up with original and valuable experimental data, which should extend our knowledge about the possibilities of improving ionic conductivity in ceramics. The outcomes of this project will be useful for researchers working not only on LTPO but also on other ceramic functional materials for energy storage and conversion.