Structure of Oxy-halide Compositions for Solid State Batteries

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Discovering new chemistry and materials to enable rechargeable batteries with higher capacity and energy density is our priorities. The novel inorganic and thermally stable oxides are potential substitutes for the toxic and flammable organic liquid electrolytes that are used in the Li-ion batteries. The oxy-halide solids are derived from the precursors of crystalline anti-perovskites of metal hydroxides and have the highest reported Li^+ and Na^+ conductivity, $\sigma > 10^{-2}$ S cm^{-1} at room temperature (25°C) [1].

Here we study Li- and Na –ion based oxides, with nominal composition: $A_xM_{1-x}O_{1+y}Cl_{1-2y}$ (where A=Li, Na and M=Ba, Ca), which were prepared from commercial precursors: NaCl, LiCl, NaOH and $Ba(OH)_2$ etc, applied multi-step heat treatments.

The structure characterization is challenging, first of all we intend to understand the atomic structure of the new materials. Neutron and X-ray diffraction experiments have been performed. Neutron diffraction experiments were carried out at the 10 MW Budapest research reactor using the PSD diffractometer, λ_0 = 1,069 Å [2]. Microstructure were analyzed on powder samples, by laboratory X-ray diffraction technique using a Brucker axs type diffractometer operating with Co Kα radiation (λ = 1,97 Å, Co Kα), stepsize was 2θ = 20-100°.

Since electrode materials are inherently nano-scale materials, local observations of these materials at high resolutions can be helpful to understand the microscopic processes that occur inside nano-particles and their interfaces with the electrolyte. Scanning electron microscopy coupled with energy dispersive X-ray spectroscopy was used to visualize and study the structural morphologies and atomic distribution. The nano-domains were verified by high-resolution transmission electron microscopy.

Neutron- and X-ray diffractions already showed that both Li and Na based compositions has a well-defined structure. All Li/Na based samples possess good hydrolytic stability, no any hydrogen bonds were detected. Details of the structural characteristics will be presented.

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References
[1] Braga M. H. *et al.* (2018) *J. Am. Chem. Soc.* **140(20)**, 6343-6352.
[2] Svab E. *et al.* (1996) *Mater. Sci. Forum* **228**, 247-252.