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Neutron diffraction study of Li diffusion in Li1+xAlxTi2-x(PO4)3 solid state lithium conductors

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Study of lithium diffusion in solid ionic conductors is a relevant part of characterization for both electrode materials and solid electrolytes for Li ion batteries. Understanding of processes supplementing lithium migration has an obvious significance for the further materials development and it was actively explored by a variety of experimental methods and techniques. While neutrons can localize light atoms in the presence of heavier ones, neutron powder diffraction is powerful tool for Li localization in the crystal structure of different compounds, which is highly relevant for understanding lithium diffusion in the materials.
All solid ceramic Li ion batteries have attracted attention as a safe, more stable alternative to conventional batteries based on liquid electrolytes, capable to operate at higher potentials. Among different materials the lithium titanium phosphate LiTi2(PO4)3 (LTP) is a promising solid-state Li+ conductor. Although LTP possesses a remarkable chemical stability against ambient atmosphere, its ionic conductivity is rather low, but it can be enhanced by partial substitution of tetravalent cations (Ti4+) by trivalent ones (Al3+, Fe3+, Y3+ etc.). The best result of the doping was obtained with aluminum, where the nominal composition Li1.3Al0.3Ti1.7(PO4)3 (LATP) was reported to have the optimum Li ionic conductivity (~10−3 S/cm) [1], thus making it promising for applications. The crystal structure is the property defining ionic conductivity and, therefore, structural properties of LATP and related materials were actively studied. Different opinions on lithium positions in LATP have been reported in the literature [2, 3]. In order to resolve these controversies a systematic neutron powder diffraction study of crystal structure of LATP–based materials was performed on the number of samples with nominally similar compositions. Careful analysis aiming to determine nuclear density maps and to define the lithium diffusion pathways was carried out on the structural data. The diffusion pathways obtained using simulations (difference bond valence) and experiment (reconstruction of nuclear density maps using maximum entropy method, MEM) have been found very similar and indicate the three dimensional Li migration in LATP which likely occurs between 6b (Li1) and 36f (Li3) sites [4].

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