Local structures and conduction pathways of Li ions for $Li_{3x}La_{2/3-x}TiO_3$ synthesized by rapid cooling

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Lanthanum titanate partly substituted lanthanum with lithium, $Li_{3x}La_{2/3-x}TiO_3$, which has a perovskite-type structure (ABO_3), exhibits the highest ionic conductivity at RT of lithium-ion conducting oxides. In the $3x$ region 0.3–0.4, furthermore, the ionic conductivity is enhanced by rapid cooling (~10^{-3} S/cm at RT) [1]. With rapid cooling, several Bragg peaks become somewhat broad in X-ray diffraction (XRD) and neutron diffraction (ND) patterns, meaning that crystal structure analyses such as Rietveld analysis and the maximum entropy method (MEM) are no longer applicable to the quenched $Li_{3x}La_{2/3-x}TiO_3$. In this work we studied three-dimensional structures and conduction pathways of Li ions for the quenched $Li_{3x}La_{2/3-x}TiO_3$ using the revers Monte Carlo (RMC) modeling and the bond valence sum (BVS) approach [2,3].

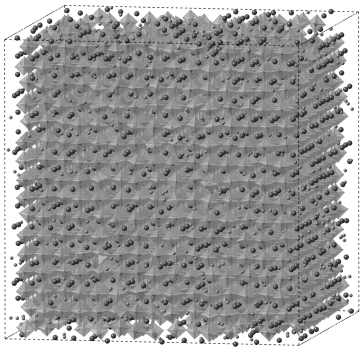

Fig. 1. Three-dimensional structure for the quenched $^7Li_{0.4}La_{0.53}TiO_3$ obtained from the RMC modeling.

The quenched $^7Li_{3x}La_{2/3-x}TiO_3$ samples with different Li contents were synthesized by solid-state reaction and rapid cooling. Their electrical conductivities were measured using four-prove ac impedance. Time-of-flight ND experiments were performed using the Neutron Powder Diffractometer NPDF at LANSCE, Los Alamos National Laboratory. Figure 1 shows the three-dimensional structure for the quenched $^7Li_{0.4}La_{0.53}TiO_3$ obtained from the RMC modeling. In the presentation we will also show the electrical conductivities and conduction pathways of Li ions predicted by the BVS approach for the quenched $^7Li_{3x}La_{2/3-x}TiO_3$.

References

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