Grain Boundary Resistance at $(La,Li)TiO_3$ Grain Boundary

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Solid-state electrolytes for Li-ion battery have advantages in thermal and electrochemical stability, and no liquid leakage that contributes a safety issue. Many materials systems have been investigated and one of promising electrolytes is $(Li_{3x}La_{2/3-x})TiO_3$ (LLTO), which has a double perovskite-type structure: La-rich and La-poor (or Li-rich) layers are alternatively stacking along the *c*-axis. In the bulk region of LLTO, Li-ion conductivity shows a significantly high as 10^{-3} S cm^{-1}, however, Li-ion conductivity in the sintered ceramics suppressed down to 10^{-5} S cm^{-1}. This abrupt reduction of ionic conductivity should be related to the grain boundary resistance, and therefore it is important to investigate the relations between the local atomic structure, chemistry and the ionic conductivity. In this study, we have investigated the atomic-structure/chemistry of polycrystalline $(Li_{0.33},La_{0.57})TiO_3$ by using atomic-resolution scanning transmission electron microscopy (STEM). On the basis of the experimental image, we also performed systematic molecular dynamic simulations.

Grain boundary analysis by electron backscattering pattern revealed that the Σ5 symmetric tilt boundary is the highest frequency in this specimen and therefore we performed atomic-resolution STEM analysis on this grain boundary. Using Z-contrast STEM imaging, we identified the La enrichment in the plane of the grain boundary, which strongly reduces the number of diffusion paths. Detailed analysis will be given in this presentation. A part of this study was supported by NEDO-RISING2 project.