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場所：本館1階H116講義室

Diffusion path of oxide ions in perovskite-type

$\text{La}_{0.64}(\text{Ti}_{0.92}\text{Nb}_{0.08})\text{O}_3$ and apatite-type $\text{La}_{9.69}(\text{Si}_{5.70}\text{Mg}_{0.30})\text{O}_{26.24}$

[Abstract]

Oxygen diffusion paths have been investigated in oxide-ion conductors $\text{La}_{0.64}(\text{Ti}_{0.92}\text{Nb}_{0.08})\text{O}_{2.99}$ with a double perovskite-type structure, and $\text{La}_{9.69}(\text{Si}_{5.70}\text{Mg}_{0.30})\text{O}_{26.24}$ with an apatite-type structure using neutron powder diffraction data by a whole-pattern fitting approach based on the maximum-entropy method (MEM). Nuclear density distribution of $\text{La}_{0.64}(\text{Ti}_{0.92}\text{Nb}_{0.08})\text{O}_{2.99}$ perovskite derived from the MEM analysis revealed that oxide ions diffused along the [100] and [010] directions near the (004) planes at 1008°C and 1358°C. On the other hand, apatite-type $\text{La}_{9.69}(\text{Si}_{5.70}\text{Mg}_{0.30})\text{O}_{26.24}$ exhibited two migration pathways at 1558 °C. One linear pathway (-O4-O4-) is parallel to the *c*-axis involving vacancy mechanism, while the other (O3-O5-O4-O5-O3) is perpendicular to the *c*-axis involving an interstitial mechanism.