Ionic Conduction Path and Disorder in $LaGaO_3$-based Fast Oxide-ion Conductors

Katsuhiro Nomura[a], Hiroyuki Kageyama[a], Masatomo Yashima[b], [a]*National Institute of Advanced Industrial Science and Technology, Ikeda, Osaka, Japan,* [b]*Tokyo Institute of Technology, Yokohama, Kanagawa, Japan.* E-mail: nomura-k@aist.go.jp

We have investigated the nuclear density distributions in $LaGaO_3$-based perovskites, $LaGaO_3$ (LG), $(La_{0.9}Sr_{0.1})GaO_{3-\delta}$ (LSG), $La(Ga_{0.9}Mg_{0.1})O_{3-\delta}$ (LGM), and $(La_{0.8}Sr_{0.2})(Ga_{0.8}Mg_{0.15}Co_{0.05})O_{3-\delta}$ (LSGMC), to elucidate the ionic conduction path and disorder of oxide ions at elevated temperatures. Neutron diffraction data were collected in the temperature range from 26 to 1405ºC in air, using a diffractometer HERMES installed at JRR-3M in JAERI (Tokai). The data obtained were analyzed by the combination technique of Rietveld analysis (using a computer program RIETAN-2000) and a maximum-entropy method (MEM)-based pattern fitting (using a computer program PRIMA). At *ca*. 1400°C, the oxide ions were localized near the equilibrium (ideal) positions for LG, while they spread over a wide area around the ideal positions for LSG and LGM. For LSGMC, the conduction path of oxide-ion was observed; the conduction path was not along the straight line between the ideal oxygen positions, but exhibited an arc shape away from the B-site cations ($Ga_{0.8}Mg_{0.15}Co_{0.05}$) [1]. The difference in nuclear density distribution is presumed to arise from the difference in oxide-ion conductivity of these compounds.

[1] Yashima M., Nomura K., Kageyama H., Miyazaki Y., Chitose N, Adachi K, *Chem*. *Phys*. *Lett*., 2003, **380**, 391.

Keywords: $LaGaO_3$, oxide-ion conduction path, maximum entropy method