Crystal Structure of Mg-doped apatite-type Ionic Conductor

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Oxygen-ionic conductors are very important materials for various kinds of applications such as fuel cells and oxygen-gas sensors. In 1995, Nakayama found new type of oxygen-ionic conductor; Ln-Si-O apatites (Ln = Lanthanoids). [1] [2] These compounds show better oxygen ionic conductivity in middle range of temperature compared with other famous oxygen-ionic conductors (ZrO_2 and/or CeO_2-based materials). Recently, Yoshioka reported that Mg-doped apatites show the best ionic conduction. [3] However, in all of the apatite system, details of mechanism of ionic conduction are still under question. In this study, we carried out powder neutron-diffraction technique to understand crystallographic details of Mg-doped Apatite-type ionic conductor.

The Mg-doped apatite-type sample was prepared by sol-gel method. [3] The chemical composition of the sample, $La_{9.7}(Si_{5.7}Mg_{0.3})O_{26.3}$, was determined by inductively coupled plasma measurements.

The neutron powder-diffraction measurement at room temperature, was carried out using IMR-HERMES diffactmetor (T1-3), installed in the JRR-3M reactor. The wavelength of neutron was 0.18265 nm, which was vertically focused by a (331) Ge monochromator. The resulting diffraction data were analyzed by the Rietveld method with RIETAN-FP [4] and whole-pattern fitting approach based on the maximum-entropy method (MPF) [5].

The Rietveld refinement was performed with neutron powder diffraction data of $La_{9.7}(Si_{5.7}Mg_{0.3})O_{26.3}$ on the basis of hexagonal $P6_3/m$. The calculated pattern agreed well with that of observed pattern. The refinement was carried out with anisotropic thermal displacement parameters for all the lanthanum sites and the oxygen sites. The final convergent indexes were Rwp = 3.68 %, Rp = 2.67 %, RR = 5.04 %, Re = 0.75 %, RI = 1.08 %, and RF = 0.46 %. The obtained cell parameters from the Rietveld analysis were a = 0.97384(3) nm, and c = 0.72140(2) nm. On the Rietveld refinement process, the interstitial oxygen positions were not able to be clearly observed. However, the oxygens may locate around the La2 site from crystallochemical point of view.

References

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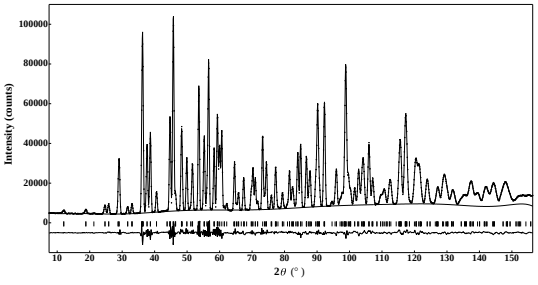

Fig. 1. Powder neutron diffraction profile of $La_{9.7}(Si_{5.7}Mg_{0.3})O_{26.3}$.