Low temperature neutron diffraction studu of (La0.8Sr0.2)ScO3-δ perovskite

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Recently, strontium doped LaScO3-based perovskites, (La1-xSrx)ScO3-δ have been investigated as the electrolyte materials of hydrogen sensors, etc., because of the relatively high proton conductivity and high chemical stability against CO2. Of these, x = 0.2 compound, (La0.8Sr0.2)ScO3-δ (LSS82) shows the highest proton conductivity of 6 × 10-3 S/cm at 873K [1]. However, the detailed crystal structure and the proton conduction mechanism of this compound are not clear. In this study, we measured the low-temperature neutron diffraction data of LSS82 between 3 and 297K, and investigated the crystal structure and the site occupation of proton.

High purity LSS82 powder was prepared by a solid-state reaction method. Obtained LSS82 powder was hold in an electric furnace at 923K for 30 hrs under wet 21%O2-79%Ar gas flow condition. The absorbed H2O content was evaluated by using a TG-MASS analyzer, and the final chemical composition was determined as (La0.8Sr0.2)ScO2.9885H0.177 (LSS82-H2O). The LSS82-H2O powder packed in a vanadium cell was set in a He gas circulating refrigerator (4K-cryo). Neutron diffraction measurements were performed with HERMES installed at JRR-3M in JAEA (Tokai) [2]. Neutron wavelength was 1.81963(4)A. Diffraction data were collected in the 2 θ range from 20 to 153 deg in the step interval of 0.1 deg, between 3 and 297K. The diffraction data obtained were analyzed by using a computer program RIETAN-2000 [3] and a maximum-entropy method (MEM)-based pattern fitting. MEM calculation was carried out using a computer program PRIMA [4].

All the reflections of LSS82-H2O between 3 and 297K were indexed by an orthorhombic symmetry (Pnma). Figure 1 shows the crystal structure of LSS82 at 3K and the speculated six hydrogen positions. Of these, the most plausible sites were H3 and H6 positions.

References

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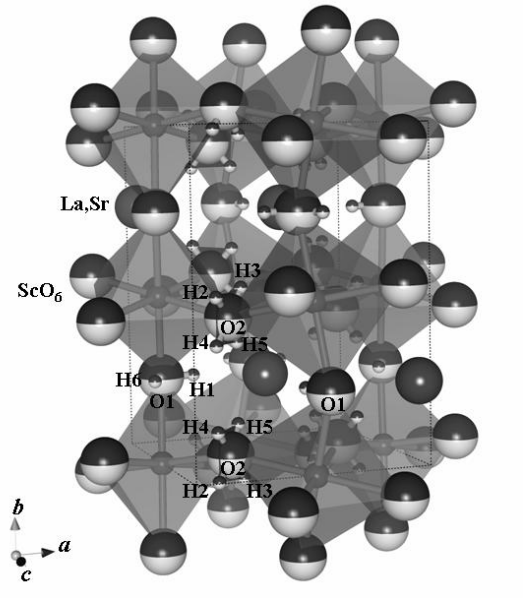

Fig. 1. The crystal structure of LSS82 at 3K and the speculated hydrogen sites. The most plausible positions: H3 and H6.