

Neutron diffraction study of SnO₂-CeO₂-SbO_x system

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Recently, SnO₂-based materials have been investigated as transparent conductive oxides, oxidation catalysts, and the sensing materials of semiconductor gas sensors [1]. Of these, as the sensing materials of sensors, SnO₂-MO_x (M = Al, Ce, etc.) systems have been mainly used. However, the detailed crystal structures of these systems are not clear yet. So far, we measured the neutron diffraction data of SnO₂-MO_x (M = Al, Ce) [2,3] and (SnO₂)₁₀₀(CeO₂)_a(SbO_x)_b (a = 1.0-3.0, b = 1.0-3.0) [4] systems, and investigated the crystal structure and the nuclear density distributions. In this study, we have investigated the crystal structure and the nuclear density distributions of (SnO₂)₁₀₀(CeO₂)_a(SbO_x)_b (a = 0.6-0.8, b = 0.6-0.8) system.

Neutron diffraction measurements of high purity (SnO₂)₁₀₀(CeO₂)_a(SbO_x)_b samples were performed with HERMES installed at JRR-3M in JAEA (Tokai) [5]. Neutron wavelength was 1.8204(5) Å. Diffraction data were collected in the 2θ range from 20 to 157 deg in the step interval of 0.1 deg. The diffraction data obtained were analyzed by the combination technique of Rietveld analysis using a computer program RIETAN-FP [6] and a maximum-entropy method (MEM)-based pattern fitting. MEM calculation was carried out using a computer program PRIMA [7].

The neutron diffraction patterns of (SnO₂)₁₀₀(CeO₂)_a(SbO_x)_b (a = 0.6-0.8, b = 0.6-0.8) samples showed larger peak widths compared to that of pure SnO₂. All the reflection peaks of these samples were indexed by a tetragonal symmetry (P4₂/mnm, No.136). The assumed structure model was as follows: Sn, Ce, and Sb atoms occupy 2a sites (0, 0, 0) and O

atoms occupy 4f sites (x, y, 0) (x = y ≈ 0.306) [1] with isotropic atomic displacement parameters. The lattice parameters and unit cell volume increased with increasing Ce and Sb contents, suggesting the introduction of larger Ce⁴⁺(0.97 Å) and Sb³⁺(0.76 Å) ions [8] into Sn⁴⁺ (0.69 Å) sites. Figure. 1 shows the equicontour surfaces (0.05 fm/Å³) of scattering amplitude of (SnO₂)₁₀₀(CeO₂)_{0.8}(SbO_x)_{0.8}. Not only 2a (Sn, Ce, Sb) sites but also 4f (O) sites showed nonspherical equicontour surfaces with larger distributions (compared to pure SnO₂), suggesting the disturbed atomic arrangements on the 2a and 4f sites by introducing Ce and Sb atoms into Sn sites.

References

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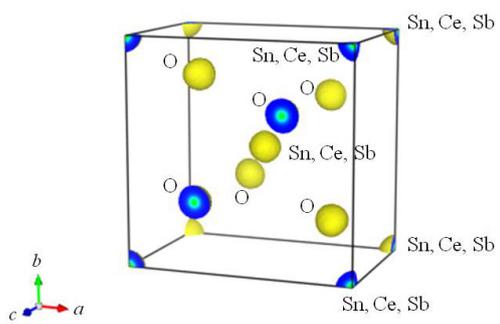


Fig. 1. Equicontour surfaces ($0.05\text{fm}/\text{\AA}^3$) of scattering amplitude of $(\text{SnO}_2)_{100}(\text{CeO}_2)_{0.8}(\text{SbO}_x)_{0.8}$