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Crystal structure of Ferroelectric Silver Niobate $AgNbO_3$

Shota Matsuyama[1], Masatomo Yashima*[2], Rikiya Sano[3], Mitsuru Itoh[4], Kenji Tsuda[3], Desheng Fu[5]
[1]Department of Materials Science and Engineering,
Interdisciplinary Graduate School of Science and Engineering, Tokyo Institute of Technology,
Nagatsuta-cho 4259, Midori-ku, Yokohama 226-8502, Japan
[2]Department of Chemistry and Materials Science, Graduate School of Science and Engineering,
Tokyo Institute of Technology, 2-12-1-W4-17, O-okayama, Meguro-ku, Tokyo, 152-8551, Japan
[3]Institute of Multidisciplinary Research for Advanced Materials, Tohoku University,
Katahira 2-1-1, Aoba-ku, Sendai 980-8577, Japan
[4] Materials and Structures Laboratory, Tokyo Institute of Technology,
Nagatsuta-cho 4259, Midori-ku, Yokohama 226-8503, Japan
[5] Division of Global Research Leaders, Shizuoka University,
Johoku 3-5-1, Naka-ku, Hamamatsu, 432-8561, Japan

Introduction

Silver niobate- ($AgNbO_3$-) based compounds are candidates for high frequency/microwave materials, overcoming the conventional $BaTiO_3$- and $PbTiO_3$-based piezoceramics. $AgNbO_3$ has a perovskite-type structure and is a lead-free material. However, the structural origins of these excellent properties of $AgNbO_3$ and $AgNbO_3$-based compounds have not been known yet. Crystal structure of ferroelectric $AgNbO_3$ was refined by the invalid *Pbcm* space group, which cannot yield the ferroelectricity. The purpose of this work is to determine the crystal structure of ferroelectric $AgNbO_3$ through the synchrotron powder diffraction [1].

Experimental

Synchrotron powder diffraction measurements were carried out at 25.1 °C by a high-angular-resolution multi-detector system [2] installed at the BL-4B$_2$ beam line of Photon Factory. The experimental data were analyzed by the orthorhombic (space group *Pmc*2$_1$) perovskite-type structure using Rietveld method with a computer program RIETAN-FP [3].

Result and Discussion

Figure 1 shows the Rietveld fitting result for the synchrotron diffraction data of *Pmc*2$_1$ $AgNbO_3$ measured at 25.1 °C (R_{wp} =8.76%, R_B =2.34%, R_F =1.47%, a = 15.64773(3) Å, b = 5.55199(1) Å, c = 5.60908(1) Å). Figure 2 shows the refined crystal structure of *Pmc*2$_1$ $AgNbO_3$ from synchrotron powder diffraction data taken at 25.1 °C. Notable feature of the crystal structure of *Pmc*2$_1$ $AgNbO_3$ is the atomic displacements along the c axis. The Nb1 displacement is larger than the Nb2 one. The Ag2 and Ag3 displacements are not equaled. Ag1 atom has a displacement. As a result, *Pmc*2$_1$ $AgNbO_3$ has a spontaneous polarization and exhibits ferroelectricity.

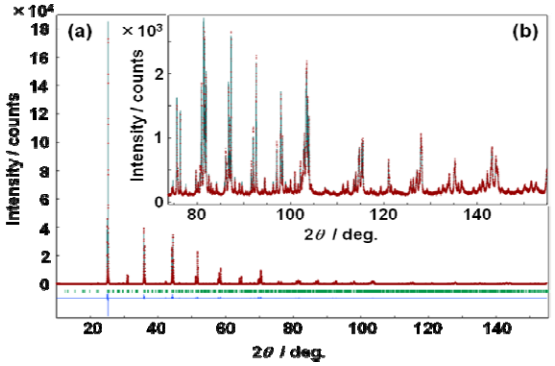

Figure 1. Rietveld fitting profiles of synchrotron powder diffraction data of *Pmc*2$_1$ $AgNbO_3$ at 25.1 °C. Wavelengths of synchrotron X-ray were 1.20825 Å. Figure (b) is an enlargement of a part of Figure (a).

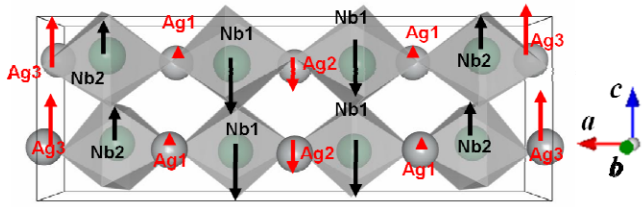

Figure 2. Refined crystal structure of *Pmc*2$_1$ $AgNbO_3$ from synchrotron powder diffraction data taken at 25.1 °C. Polyhedron stands for an NbO_6 octahedron. Gray and green balls stand for Ag and Nb atoms, respectively. Red and black arrows stand for the displacements of Ag^+ and Nb^{5+} ions, respectively.

References

[1]M. Yashima, S. Matsuyama, R. Sano, M. Itoh, K. Tsuda, and D. Fu. Chem. Mater. 23, 6 (2011).
[2]H. Toraya, H. Hibino, K. Ohsumi, J. Synchrotron Rad. 3, 75 (1996).
[3]F. Izumi and K. Momma, Solid State Phenom. 130, 15 (2007).
* yashima@cms.titech.ac.jp