Structural analysis of multiferroic perovskite-type $YMnO_3$ single crystal

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Multiferroic materials have been intensively studied, focusing on the interests in the driving mechanism of cross-correlated interactions between the magnetism and electricity [1]. Many theoretical and experimental works have clarified the origin of the interplay between magnetism and electricity. However, the lack of information about the crystal structure in the multiferroic phase has prevented quantitative discussion of the ferroelectricity driven by magnetic order. In order to quantitatively discuss the microscopic origin of the ferroelectricity of multiferroic perovskite-$YMnO_3$, in which the $\uparrow\uparrow\downarrow\downarrow$-type ($E$-type) antiferromagnetic order causes a ferroelectric polarization below 30 K [2], we performed the crystal structural analysis for a twin-free single crystal by using synchrotron x-ray diffractometer at BL02B1 in SPring-8, and successfully determined the atomic displacements associated with the ferroelectric order. The space group of the multiferroic phase is $P2_1nm$, which is consistent with that expected for the exchange striction mechanism giving rise to a ferroelectric polarization along the a-axis. From the experimental results of magnetization, electric polarization, permittivity, and infrared spectrum in addition to x-ray diffraction and a theoretical first-principles calculation, we quantitatively discuss the ferroelectricity in multiferroic $YMnO_3$.

[1] Y. Tokura and S. Seki, Adv. Mater. **22**, 1554 (2010).

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