Crystal Structure Refinement of Sr(Mg_{1/3}Nb_{2/3})O₃

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Generally a perovskite compound undergoes the phase transition through a cation substitution originating by ordering and tilting phenomena. Barium magnesium niobate, Ba(Mg_{1/3}Nb_{2/3})O₃ (BMN) are typical compounds which have revealed 1:2 ordered structures with the trigonal symmetry. As the La substituted, the structure undergoes the phase transition by cubic, monoclinic[1,2]. In this paper, we present the structural changes in accordance with the cation substitution of Sr by using neutron Rietveld refinement. Neutron powder diffraction data of the sample was obtained at room temperature using high resolution powder diffraction at Korea Atomic Energy Research Institute. The structure model of SMN was used the results deduced from the HRTEM experiments, which SMN has the antiphase tilting and 1:2 ordering. From the refinement, SMN has the monoclinic structure which has 1:2 ordering and antiphase tilting. The space group was determined to be C2/m (#12) with $a(\text{\AA})=9.8042(2)$, $\hat{b}(\text{\AA})=13.7954(2), c(\text{\AA})=5.6310(1), \beta=90.145(2)^{\circ}, V=761.60(3)\text{\AA}^3$. The structure of SMN is distorted by the antiphase tilting of oxygen octahedral with the a^ob-b- system of the (MgNb)O₆ polyhedra.

[1] Park H. M., et al., *J. of Material Research*, 2003, **18(4)**, 1003-10. [2] Park H. M., et al., *Materials Research Bulletin*, 2001, **40(6)**, 1021-33. Keywords: perovskite, antiphase tilting, crystal structure