MLF Experimental Report	提出日 Date of Report September 18, 2013
課題番号 Project No. 2013A0136 実験課題名 Structural Origin of the Visible-Light Response of the Metal Oxynitride Photocatalysts. Band Gap-Structure Correlation 実験責任者名 Name of principal investigator Masatomo Yashima 所属 Affiliation Department of Chemistry and Materials Science, Graduate School of Science and Engineering, Tokyo Institute of Technology	装置責任者 Name of responsible person Toru Ishigaki 装置名 Name of Instrument/（BL No.） BL-20 実施日 Date of Experiment May 7-9, 2013

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。（適宜、図表添付のこと）
Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.

ANbO$_2$N photocatalyts (A: Ba, Sr), $AA'BO_4$- and $A_x\,A'_y\,B_zO_w$-based materials (A, A': large cations such as rare earth La, Pr, Nd, Y, Ho, Er, Yb and Ba, Sr, Ca; B: smaller cations as Al, In, Ga, Co, Sn).

2. 実験方法及び結果（実験がうまくいかなかった場合、その理由を記述してください。）
Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.

Experimental methods

Due to the radioactive material leak accident of the Hadron Experimental Facility of J-Parc, we were able to do only 30% of the experiments of this proposal. Neutron powder diffraction data of ANbO$_2$N photocatalyts, $AA'\,BO_4$- and $A_x\,A'_y\,B_zO_w$-based materials were measured at room temperature by a high-resolution neutron powder diffractometer iMateria installed at the beam line BL20 of J-Parc facility, Japan. The sintered or the powdered samples were put into 6 mmϕ vanadium sample holders and were used for the diffraction measurements. The diffraction data were analyzed by the Rietveld method with a computer program Z-Rietveld.

Experimental results

Rietveld analysis of BaNbO$_2$N photocatalyst (Figure 1) indicates the cubic perovskite-type structure, while SrNbO$_2$N photocatalyst was successfully analyzed by the tetragonal structure. The reduced unit-cell volume of

2. 実験方法及び結果（つづき） Experimental method and results (continued)

$SrNbO_2N$ is smaller than that of $BaNbO_2N$. The interatomic distances of $SrNbO_2N$ are shorter than those of $BaNbO_2N$.The lower symmetry, smaller reduced cell volume and shorter interatomic distances of $SrNbO_2N$ are attributable to the smaller ionic size of Sr^{2+} compared with Ba^{2+}, leading to lower tolerance factor. The Nb-(O,N)-Nb' angle of $BaNbO_2N$ is 180°. The Nb-[equatorial (O,N)]-Nb' angle of $SrNbO_2N$ is 180°, while the Nb-[apical (O,N)]-Nb' angle of $SrNbO_2N$ is estimated to be 172.48(6)°. The lower Nb-[apical (O,N)]-Nb' angle may make less overlapping of Nb and (O,N) orbitals, which leads to wider band gap. In fact, the band gap of $SrNbO_2N$ is known to be wider than that of $BaNbO_2N$.

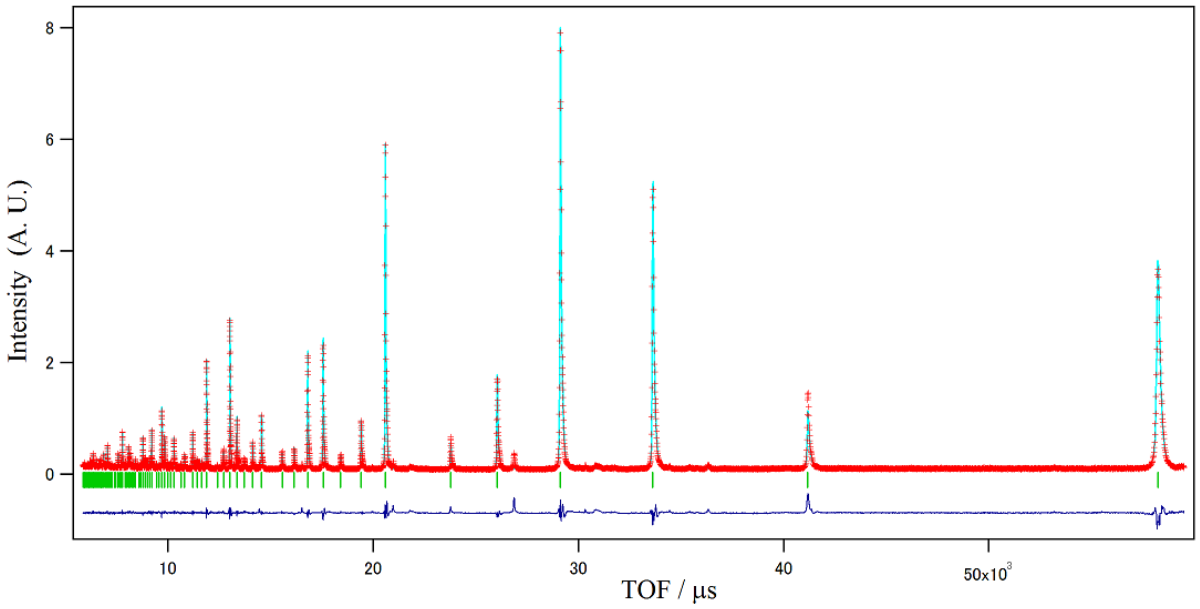

Figure 1. Rietveld pattern of neutron powder diffraction data of $BaNbO_2N$ taken at room temperature.