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Space Group Determination of the Magnetically Induced Ferroelectric Phase of Multiferroic YMn_2O_5

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1 Introduction

Multiferroic YMn_2O_5 belongs to a centric space group *Pbam* and shows paraelectric properties at RT, and the spontaneous polarization grows along a b-axis about 40K by cooling [1]. Although the atomic displacement pattern, which might originate the spontaneous polarization, is one of the most significant and interesting topics of structural science of YMn_2O_5, even the space group symmetry in the ferroelectric phase is not determined yet without ambiguity. In our previous study at PF4C and SPring-8 BL02 using a four-circle diffractometer, super lattice reflections indicating the formation of twice as large unit cell along the *c*-direction referred to the paraelectric phase were observed. However, since the contributions of the displacements to diffracted intensities are so small and easily contaminated by false intensities of multiple diffractions, space group determination was not fully succeeded at that time. This time, applying psi-rotation method and changing photon energy to avoid simultaneous reflections, we tried space group determination again.

2 Experimental

Single crystals of YMn_2O_5 were grown by the flux method and grinded into sphere of 245 μm in diameter and used for X-ray diffraction measurement at BL14A. Psi-scan simulation software MCD++ was prepared and optimum four-circle angles setting to avoid simultaneous reflection condition were calculated for every reflection. All the diffracted intensities were measured at the calculated angles using the four-circle diffractometer installing avalanche photodiode (APD) detector whose count loss is less than 1% up to 10^7 cps. Compressed cold helium gas was directly flowed onto the specimen to cool the sample. Temperature dependencies of diffracted intensities of extinction-reflections in paraelectric phase and superlattice reflections were measured around ferroelectric transition temperature. Since the diffracted intensities of these reflections are more than 10^6 times less than that of the strongest one, complete avoidance of multiple reflections are not easy.

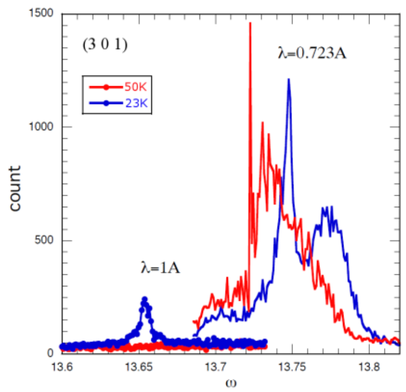

Figure 1: Peak profiles of (3 0 1) reflections above and below *Tc* for different incident X-ray wavelengths λ=1Å and λ=0.723Å. ; 23K in blue, 50K in red.

Figure 1 shows peak profiles of (3 0 1) reflections above and below the transition temperature and exhibits that contamination in 1.0 Å is much less than in 0.723 Å. Therefore, testing with various wavelengths is crucially important to judge the observed peak is real one or spurious one.

3 Results and Discussions

Figure 2 shows a part of the results. A superlattice reflection (0 0 4.5) and an extinction-reflection (3 0 1) in paraelectric phase are shown, and temperature dependency of these two are synchronize below the transition temperature. From these, the space group of ferroelectric phase should be $Pb2_1m$ which removed the *a*-glide plane from *Pbam*. An extinction reflection due to *b*-glide planes vertical to ***a*** (0 5 5) is also observed with this wavelength but shows no temperature dependency, thus, this is ascribed to simultaneous reflections.

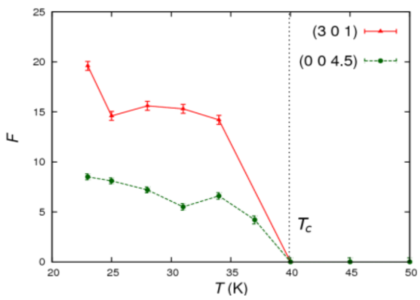

Figure 2: Temperature dependency of diffracted intensities; superlattice reflection (0 0 4.5), and extinction-reflection at RT due to *a*-glide planes vertical to ***b*** (3 0 1). Relatively lower energy of 0.85 angstrom X-ray was used.

References
[1] M.Fukunaga, et.al, JPSJ **79**, 054705 (2010)
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