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Effect of Orbital State on Anisotropic Scattering Factor Tensor

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Introduction

Resonant x-ray scattering (RXS) allows us to detect the pattern of periodic local symmetry belonging to a specific element through the anisotropy of the atomic form factor. Recently this technique has been applied to orbital-ordered Mn oxides [1] in order to determine their electronic states, i.e., charge ordering or orbital ordering. However, quantitative analysis of the RXS signal has been difficult because the relationship between the anisotropy of the electron cloud and that of the form factor used in RXS experiments is unclear.

For the K-edge RXS, the anisotropy reflects that of the Mn 4*p* level. There are two theoretical explanations for the 4*p* anisotropy. One is that the Jahn-Teller (JT)-mode lattice distortion affects the 4*p* level [2]; we call this mechanism the ``JT mechanism". The other is the electrostatic effect due to the anisotropic 3*d* electron cloud [3]. We call this the ``Coulomb mechanism". Experimentally, it was already shown that the JT mechanism is greater than the Coulomb mechanism [4,5]. In this study, we obtain the ratio of the two effects.

Experiment

Samples

In order to control the degree of lattice distortion, we chose thin films as the samples. The samples we measured were $SrMnO_3$, $La_{0.6}Sr_{0.4}MnO_3$, $Pr_{0.6}Sr_{0.4}MnO_3$, and $Nd_{0.6}Sr_{0.4}MnO_3$ films on $SrTiO_3$ (001) substrate; we will abbreviate them as SMO, LSMO, PSMO, and NSMO, respectively. SMO does not have anisotropic e_g electrons while the other films have e_g electrons. The thickness of SMO was 200A and those of the others were 600A. Epitaxial samples were fabricated by means of a pulsed laser deposition method.

Structure estimation

In order to separate the JT mechanism component from the total anisotropy of the form factor, we have to obtain the degree of JT distortion for all the samples. X-ray diffraction measurements with x-rays having energies near the La, Pr, Nd, and Mn absorption edges were made at BL1A and 9C in order to obtain the contribution of the element to a reflection. This provides the systematic extinction of each element and reduces the number of free structure parameters; this is a traditional RXS experiment. This technique was used to cover the small number of observed reflections. We obtain the atomic position with assuming the space group *Pbnm*, which is the space group usually seen in bulk manganites.

Resonant X-ray Scattering

The anisotropy of the form factor was obtained at BL9C by the interference method [4]. The anisotropy of SMO denotes the anisotropy caused by JT mechanism. The other samples have both Coulomb and JT components. With assuming that the JT component is proportional to the degree of JT distortion, one can obtain the Coulomb components.

Results and Analysis

The structure of SMO was found to be the $StTiO_3$ structure with a compression along *c*-axis. RXS measurements on the other three films shows that LSMO has no atomic displacements of La, while NSMO and PSMO have finite atomic displacements of Nd or Pr within orthorhombic *b*-direction. Using 7 unique superlattice intensities for LSMO and 27 for NSMO and PSMO, we obtained the degree of JT distortion as shown in abscissa axis of Fig.1. Obtained anisotropy of the form factor is also shown in Fig.1. The JT component was obtained as the solid line and the Coulomb component is the difference between the plot and the line. Our result shows that the Coulomb component is smaller than experimental error. Detailed discussion is given in Ref. [6].

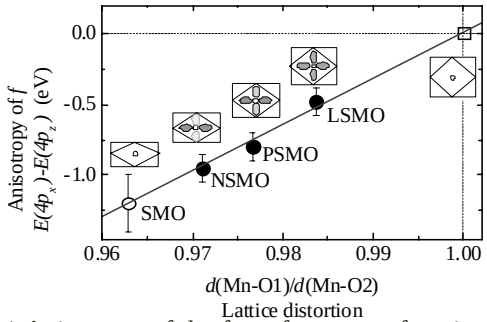

Fig.1 Anisotropy of the form factor as a function of the degree of JT distortion.

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