Type of presentation: Poster

IT-5-P-2570 Orbital ordering of A-site ordered $SmBaMn_2O_6$ studied by inelastic scattering accampanied by Mn-L shell excitation

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Manganite perovskites have been drawing a grate attention from the unique properties such as metal-insulator transition, colossal magneto-resistance, etc. Such unique properties are attributed to a charge and orbital ordering (COO) of the 3*d* electrons in the e_g orbitals of Manganese by resonant X-ray scattering experiments. $SmBaMn_2O_6$ shows the A-site ordering of Sm and Ba at room temperature. The crystal structure has a $2\sqrt{2}a_p \times 2\sqrt{2}a_p \times 4a_p$ supercell with a_p the fundamental cubic perovskite unit cell reported. In the present study, we determine the orbital ordering of $SmBaMn_2O_6$ by the convergent-beam electron diffraction (CBED) and inelastic scattering [3] accompanied by Mn-*L* shell excitation.

Samples of $SmBaMn_2O_6$ were synthesized by a solid-state reaction using Sm_2O_3, $BaCO_3$, and MnO_2. CBED patterns were taken from an area of about 10 nm in diameter. Inelastic scattering patterns accompanied by the Mn-*L* shell excitation were taken using an energy-filtering system fitted to the bottom of the electron microscope. A series of inelastic scattering patterns at successive energy losses from 620 eV to 670 eV with an energy step of 1-2 eV were taken with an energy window of 1-2 eV.

Figures 1(a), 1(b) and 1(c) show CBED patterns of $SmBaMn_2O_6$ taken at incidences in the [0 0 1], [0 1 0] and [0 4 1] orientations, respectively. The [0 0 1] and [0 1 0] patterns show two types of mirror symmetries and twofold rotation symmetry. Thus, the point group is determined to be *mmm*. The patterns does not show any systematic extinction rules of reflections, indicating that the lattice type is primitive *P*. From the dynamical extinction lines in the *h*00 (*h* = odd) reflections in the [0 0 1] pattern and 0 -4 17 reflection in the [0 4 1] pattern, the space group of $SmBaMn_2O_6$ was determined to be *Pnam*.

Figure 2(a) shows an inelastic scattering pattern of $SmBaMn_2O_6$ accompanied by the Mn-*L* shell excitation taken at an incidence in the [0 1 0] orientation. The pattern clearly shows an elongation along the *a** axis. Figures 2(b) and 2(c) show inelastic scattering patterns simulated from two kinds of the orbital ordering composed of the $3z^2$-r^2 type orbitals [1] and the x^2-y^2 type orbitals [2], respectively. The anisotropic feature of the experimental inelastic scattering patterns agrees well with that of the x^2-y^2 type model. An orbital-ordering model was constructed from the CBED symmetry and a qualitative comparison between the experimental and simulated inelastic scattering anisotropy.

References

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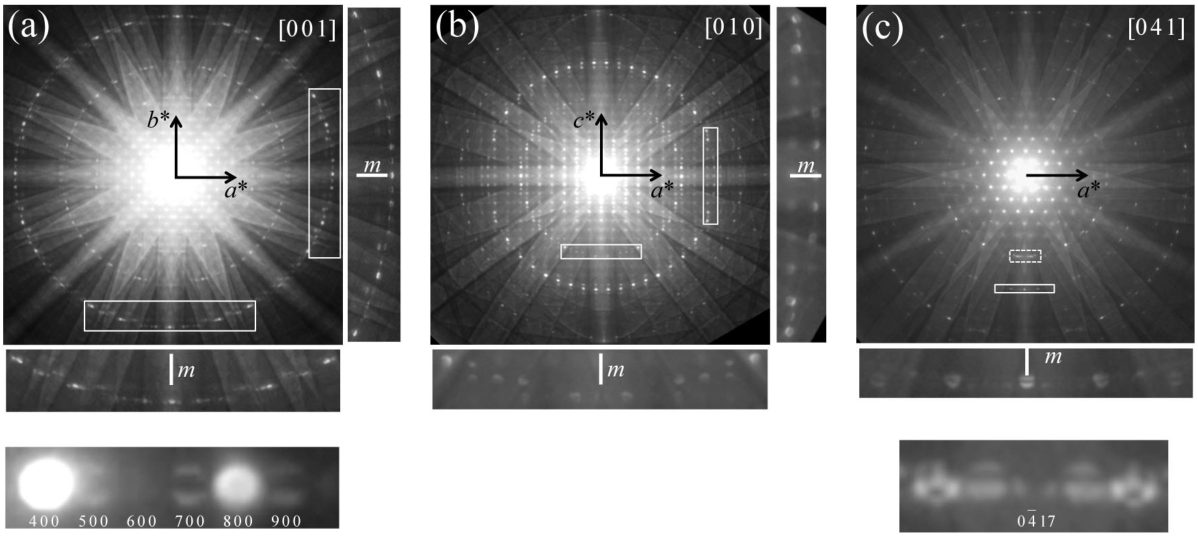

Fig. 1: Convergent-beam electron diffraction patterns of $SmBaMn_2O_6$ taken at incidences in the [0 0 1], [0 1 0] and orientations. The and patterns show two types of mirror symmetries and twofold rotation symmetry. Dynamical extinction lines in the [0 0 1] and [0 -4 17] patterns indicate that there exist a and n glide planes.

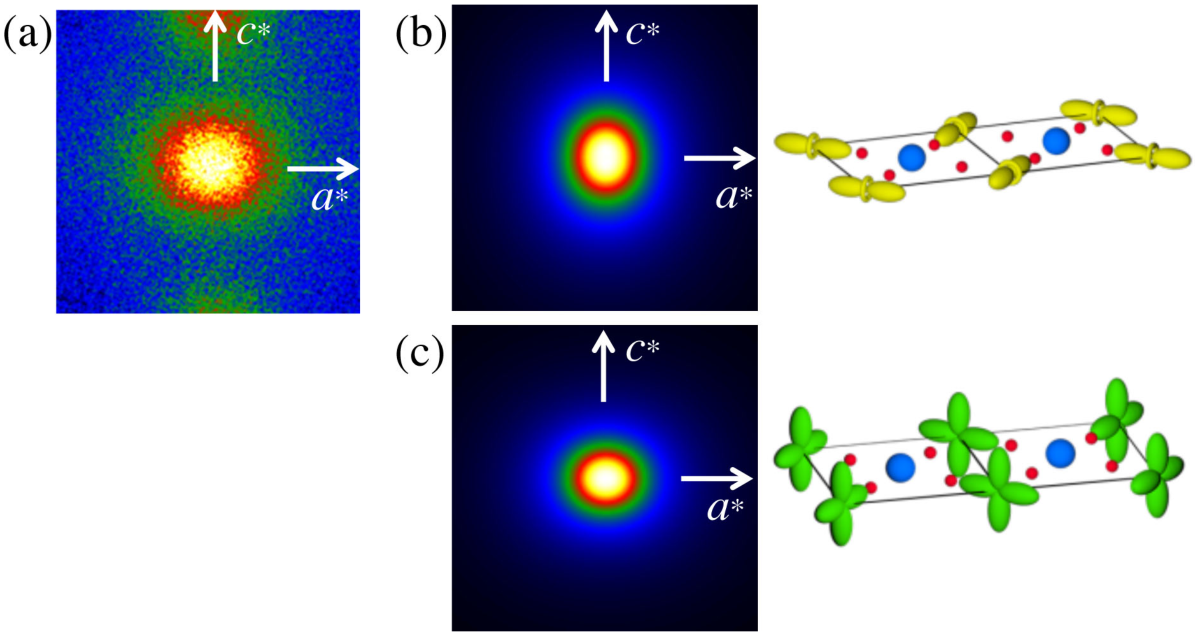

Fig. 2: Experimental inelastic scattering pattern of $SmBaMn_2O_6$ accompanied by Mn-L shell excitation taken at an incidence in the [010] orientation (a) and simulated patterns from the $3z^2$-r^2 orbital model (b) and the x^2-y^2 orbital model (c). The elongation feature in the experimental pattern agrees well with the pattern simulated from the x^2-y^2 model.