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Effects of Madelung potentials in the photoemission spectra of $La_{1-x}Sr_xMnO_3$ thin films

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Introduction

The binding energy of a core level observed by photoemission spectroscopy is determined by a lot of factors. The shift ΔE of the energy of a core level measured relative to the chemical potential μ, when the band filling is varied and/or the crystal structure is changed, is given by [1]

$\Delta E = -\Delta\mu + K\Delta Q - \Delta V_M + \Delta E_R$,

where $\Delta\mu$ is the change in the chemical potential, ΔQ is the change in the number of valence electrons on the atom, K is a constant, ΔV_M is the change in the Madelung potential and ΔE_R is the change in the extra-atomic relaxation energy of the core–hole state. When the band filling is varied, both μ and V_M changes, but the effect of ΔV_M has not been observed so far [2]. In this study, we investigate the effect of V_M from the core-level photoemission spectra of $La_{0.6}Sr_{0.4}MnO_3$ (LSMO) thin films grown on various substrates [3, 4]. By fixing the Sr composition, one can extract the information of ΔV_M with keeping the other terms constant.

Experiment and calculation

The LSMO thin films were fabricated in a laser MBE chamber and transferred in vacuum to a photoemission chamber at BL-2C of the Photon Factory [5]. The films were grown on $LaAlO_3$ (LAO) (001) (with compressive strain), $(LaAlO_3)_{0.3}$-$(SrAl_{0.5}Ta_{0.5}O_3)_{0.7}$ (LSAT) (001) (with almost no strain), and $SrTiO_3$ (STO) (001) (with tensile strain). The lattice constants determined by four-circle x-ray diffraction were summarized in Table 1. The values of Madelung potentials were calculated by Ewald's method.

Table1: In-plane (a-axis) and out-of plane (c-axis) lattice constants of LSMO thin films grown on LAO, LSAT and STO substrates.

Substrates	a (Å)	c (Å)	c/a
LAO	3.79	3.98	1.05
LSAT	3.87	3.87	1.00
STO	3.91	3.83	0.98

Results and Discussion

Figure 1 shows the binding-energy shifts of each core level in LSMO thin films obtained by experiment (photoemission spectroscopy) (a) and calculation (b). First we notice that the energy scales of the shifts are similar (~ 100 meV) in both experiment and calculation. In O 1s, the Madelung potentials felt by in-plane and out-of-plane O atoms are quite different, but we do not observe such splitting in the O 1s core-level photoemission spectra. As seen from Fig. 1 (a), the experimental shifts of O 1s and Mn 2p are negligible, inconsistent with the calculation in Fig. 1 (b). As for Sr 3d and La 4d, the experimentally observed shifts in Fig. 1 (a) are almost the same as the calculation in Fig. 1 (b). These different behaviors can be explained by the existence of valence electrons. In O and Mn atoms, the valence electrons (O 2p and Mn 3d) are redistributed to screen the effects of Madelung potential, thus keeping the binding energy of core levels almost constant. La and Sr atoms do not have such valence electrons, and the effects of Madelung potential are unscreened and directly reflected in the core-level photoemission spectra. This scenario is also consistent with the negligible effects of ΔV_M when the band filling is varied. In the case of band filling, the doped carriers are uniformly distributed and ΔV_M is kept almost zero in all core levels.

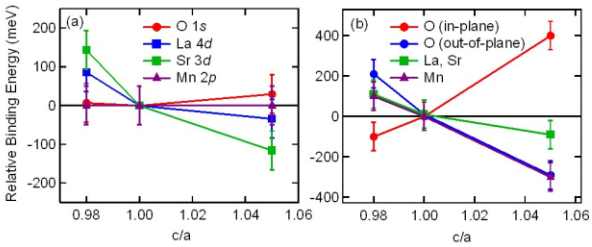

Fig. 1: Binding-energy shifts of each core level in LSMO thin films. (a) Experimental values determined by photoemission spectroscopy. (b) Calculated values determined from the effect of ΔV_M.

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