Coherent and incoherent band dispersions in V 3d band of SrVO₃ thin films

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Introduction

Metal-insulator transition has been extensively studied because of its fundamental importance as well as its close relationship to interesting phenomena such as hightemperature superconductivity in cuprates and colossal magnetoresistance in manganites [1]. Ca_{1,x}Sr_xVO₃ (CSVO) is a typical bandwidth control system but remains metallic in the entire x range. With Ca doping, ultra-violet photoemission spectra of CSVO showed spectral weight transfer from the coherent part to the incoherent part [2], while using high photon energies there were no spectral weight transfer [3]. Therefore, it is now well known that the surface electronic states are different from the bulk ones. Many studies were devoted to investigate the real "bulk" electronic states [4-6], but the problem remains highly controversial and further studies are strongly required. In the present work, we have fabricated a SrVO₃ (SVO) thin film and studied its electronic structure in detail by angle-resolved photoemission spectroscopy (ARPES).

Experiment

A SVO thin film was fabricated in a laser MBE chamber connected to a synchrotron radiation ARPES system at BL-28B of Photon Factory [7]. The films were deposited on Nb-doped TiO₂-terminated SrTiO₃ (001) substrates [8] at 900 °C at an ultra high vacuum of ~10⁻⁹ Torr. The fabricated SVO thin film was transferred into the photoemission chamber under an ultrahigh vacuum of 10^{-10} Torr. The ARPES spectra were taken at 20 K with the total energy resolution of 30 meV.

Results and Discussion

The $E - k_x$ space intensity plot near E_F along the $\Gamma - X$ direction in Fig. 1 shows the V 3*d* bands. The peak positions determined from both energy distribution curves (EDCs) and momentum distribution curves (MDCs) are also shown. The V $3d_{xy}$ and $3d_{zx}$ bands cross the Fermi level between the Γ and X points. For the dispersion of the coherent part, one can see clear mass renormalization compared with the LDA calculation [9]. From the experimental (-0.44 ± 0.02 eV) and calculated (-0.95 eV) occupied bandwidths, the global mass renormalization factor is estimated to be ~ 2. That is, if the LDA band dispersions are reduced by a factor of 0.5, the experimental band dispersions are well reproduced as shown in Fig. 1. This indicates that the self-energy is nearly independent of momentum and of the d_{xy} , d_{yx} or d_{zx}

bands of the degenerate t_{2g} band. The kink in the band dispersion is weak and broad, if exists, but the curvature changes its sign around ~ -0.2 eV as predicted by a recent DMFT calculation [10]. As for the incoherent part located around -1.5 eV, one can see a weak but finite (~ 0.1 eV) dispersion. The intensity of the incoherent part is momentum dependent and becomes strong within the Fermi surface.



Figure 1: Energy- and momentum-dependent spectral weight near the Fermi level for $SrVO_3$. Peak positions of the EDCs and MDCs are shown by filled circles and open squares, respectively. The V 3*d* bands from the LDA calculation [9] is also shown by solid curves. Broken curves are LDA bands renormalized by a factor of 2.

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