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Angle-resolved photoemission study of SrVO$_3$ and CaVO$_3$

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Introduction

Strongly correlated $3d$ electrons in transition metal oxides (TMO's) has been one of the most fundamental issues in condensed matter physics [1] because the complex nature of the correlated electrons causes various interesting phenomena such as high-T_c superconductivity. Among TMO's, light transition-metal oxides such as perovskite-type Ti and V oxides are ideal systems to study the prototypical Mott-Hubbard-type systems. The issue of mass renormalization and spectral weight transfer caused by electron correlation has been controversial for the bandwidth-control Mott-Hubbard system Ca$_{1-x}$Sr$_x$VO$_3$ (CSVO). The early photoemission results have shown that, with decreasing x, i.e., decreasing bandwidth, spectral weight is transferred from the coherent part to the incoherent part [2]. In contrast, a recent ``bulk-sensitive'' photoemission study using soft X-rays have found that there is no appreciable spectral weight transfer between SrVO$_3$ and CaVO$_3$ [3]. However, a very recent ``bulk-sensitive'' laser photoemission study has revealed a suppression of spectral weight near E_F in going from SrVO$_3$ to CaVO$_3$ [4]. These discrepancies between the different experiments may stem from the difficulty in disentangling overlapping surface and bulk signals in the photoemission spectra. In order to overcome this difficulty, direct observation of the electronic structure of correlated bulk materials is desired. Previously, we have observed band dispersions and Fermi surfaces of SrVO$_3$ by angle-resolved photoemission spectroscopy (ARPES) [5]. In this work, we have performed ARPES study of SrVO$_3$ and CaVO$_3$ to observe the band dispersion near the Fermi level and directly compared the renormalization of their band width.

Experiment

ARPES measurements were performed at Beamline 28A of Photon Factory with a Scienta SES-2002 electron analyzer. The typical energy and angular resolutions were about 30 meV and 0.3 degree, respectively. Single crystals of SrVO$_3$ and CaVO$_3$ were grown using the travelling-solvent floating zone method. Samples were first aligned *ex situ* using Laue diffraction, cleaved *in situ* along the cubic (100) surface at a temperature of 20 K and measured at the same temperature.

Results and Discussions

Figure 1 of the upper panels show ARPES spectral weight measured using the photon energy hν=85 eV in the momentum-energy space. The measured momentum region is near the Γ point and the momentum direction is the V-O bond direction. The observed parabolic band is d_{xy} band which has nearly two-dimensional electronic structure along the sample surface. Spectral features of CaVO$_3$ are broader than that of SrVO$_3$, which may be due to the orthorhombic crystal distortion in CaVO$_3$. Lower panels are the second derivative plots of the energy distribution curves (EDC's) corresponding to the upper panels. The binding energy of the bottom of the band for CaVO$_3$ is ~0.4 eV, which is smaller than that for SrVO$_3$ ~0.5 eV. The narrower band width of CaVO$_3$ than that of SrVO$_3$ is consistent with the results of the band calculation [6] and is due to the distorted V-O-V bond angle in CaVO$_3$. However, the observed band widths for both samples are almost half of that predicted by the band structure calculation [6], which indicates the mass renormalization caused by the electron correlation.
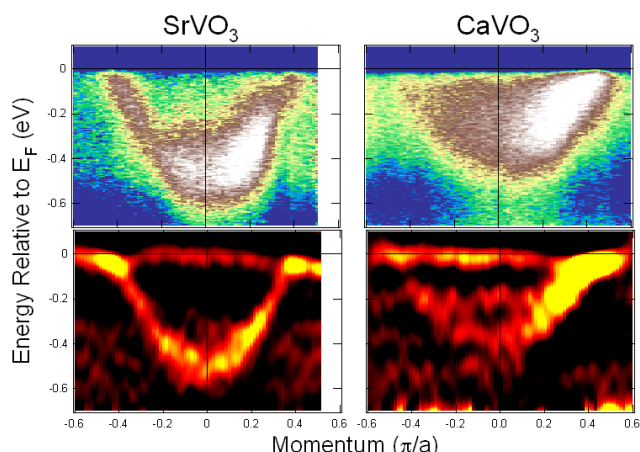

Figure 1: d_{xy} band of SrVO$_3$ and CaVO$_3$ observed by ARPES. Upper panels and lower panels indicate the ARPES intensity and the second derivative plots, respectively.

References

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