

Thickness dependent electronic structures of SrVO₃ thin films studied by *in situ* photoemission spectroscopy

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Introduction

Metal-insulator transition (MIT) is one of the most interesting phenomena in solid-state physics. According to Mott-Hubbard theory, MIT can be controlled by the relative magnitude of on-site Coulomb repulsion U and bandwidth W .

Sr_{1-x}Ca_xVO₃ (SCVO) is a typical $3d^1$ perovskite material whose bandwidth W is controlled by the Ca concentration x , owing to the change of the V-O bond length and V-O-V bond angle. However, SCVO shows the metallic behavior in all Ca concentrations [1], and MIT has not been reported in bandwidth controlled SCVO.

We have proposed a new approach for controlling W using digitally controlled film form. Since the decrease of film thickness causes the reduction of effective coordination number, the resultant reduction of effective W may drive the MIT in SVO. Here we report the spectral evidence for MIT in digitally controlled SVO thin films using photoemission spectroscopy.

Experiment

Digitally controlled SVO thin films were fabricated onto the Nb doped SrTiO₃ (Nb-STO) substrates in a laser molecular-beam epitaxy chamber connected to a synchrotron radiation photoemission system at BL2C. SVO thin films were deposited at the substrate temperature of 900 °C under an ultrahigh vacuum of 10⁻⁸ Torr. The film thickness was controlled by monitoring the intensity oscillation of the specular spot in RHEED during growth. The crystal structures of the epitaxial SVO thin films were characterized by four-circle x-ray diffraction measurement. The in-plane lattice constant of SVO thin films matched perfectly with that of STO substrates. The atomically flat surfaces with step-and-terrace structures were observed in the AFM image.

Results and Discussion

Figure 1 (a) shows the valence band spectra of SVO thin films with varying film thickness. The valence band spectra in the binding energy range from 9.0 eV to 3.0 eV mainly consist of O $2p$ derived states, while the V $3d$ derived states are seen in the band gap of STO [from 3.0 eV to the Fermi level (E_F)]. In order to investigate these V

$3d$ derive states in great detail, we have taken spectra near E_F as shown in Fig. 1 (b). The V $3d$ band consists of two components: one is the coherent (quasiparticle) part located near E_F and the other is the incoherent part located at 1.5 eV below E_F which is the remnant of the lower Hubbard band. With increasing SVO film thickness, spectral weight is transferred from the incoherent part to the coherent part. MIT occurs at about 4-5 ML of SVO thickness. On the other hand, the peak position of the incoherent part seems to remain unchanged. This means that U is independent on the film thickness of SVO. These results suggest that the observed MIT is caused by the reduction in magnitude of W due to the dimensional crossover.

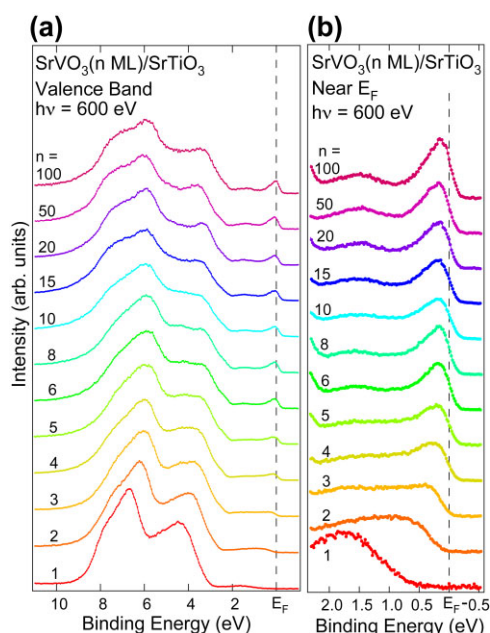


Figure 1 (a) Valence band spectra and (b) spectra near the Fermi level of SrVO₃ thin films with varying thickness.

References

[1] A. Sekiyama *et al.*, Phys. Rev. Lett. **93**, 156402 (2004).

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