Dimensional-Crossover-Driven Metal-Insulator Transition in SrVO₃ Ultrathin Films Studied by in situ Photoemission Spectroscopy

We have investigated the changes occurring in the electronic structure of SrVO₃ ultrathin films across the dimensionality-controlled metal-insulator transition (MIT) by in situ photoemission spectroscopy. With decreasing film thickness, an energy gap is formed at $E_F$ through spectral weight transfer from the coherent part to the incoherent part, indicating the MIT in the SrVO₃ ultrathin film. The observed spectral behavior is reproduced by layer dynamical-mean-field-theory calculations, and it indicates that the observed MIT is a Mott-transition caused by the reduction in the bandwidth due to the dimensional crossover in the presence of electron correlations.

Metal-insulator transition (MIT) is one of the most fundamental phenomena in condensed matter physics [1]. According to the Mott-Hubbard theory [2], MIT can be controlled by varying the relative magnitudes of on-site Coulomb repulsion $U$ and bandwidth $W$. Thus, in the case of bulk materials, MIT has been intensively studied by chemical substitution of constituent ions with ones having a smaller ion radius, where $W$ is controlled by the resultant changes in the bond angle between transition metal ions and oxygen ions. However, such chemical substitutions always induce randomness in a solid, and consequently this unavoidable chemical disorder has considerably obscured the nature of MIT induced by bandwidth control [3].

Here, we propose an alternative approach to study bandwidth controlled MIT, using dimensional crossover occurring in an artificial structure. Since a decrease in the layer thickness of ultrathin films causes a reduction in the effective coordination number of constituent ions at the interface and surface, the resultant reduction of the effective $W$ from a three-dimensional (3D) thick film to the two-dimensional (2D) ultrathin film may drive MIT in the conductive transition metal oxides.

We have applied this new approach to a typical perovskite material with 3D configuration, SrVO₃ (SVO). An SVO ultrathin film is an ideal system for studying the dimensional-crossover-driven MIT, because of the robust metallic states in SVO, irrespective of chemical substitutions. By using a digitally controlled film form, we first observed the MIT induced by the dimensional crossover in SVO ultrathin films by employing in situ photoemission spectroscopy [4].

![Figure 1](image1.png)

Figure 1 (a) shows the symmetrized V 3d spectra of SrVO₃ ultrathin films grown onto Nb:STO substrates by digitally controlling the SVO layer thickness. In the case of thicker SVO films, there are two components in V 3d spectra: a peak located at the Fermi level ($E_F$) and a relatively broad peak centered at about 1.5 eV that corresponds to the coherent (quasiparticle peak) and incoherent (the remnant of the lower Hubbard band) parts, respectively. With decreasing film thickness, the spectral weight is transferred from the coherent to the incoherent part in the layer thickness of 3–6 ML, and finally the V 3d spectra for the film thicknesses of 1–2 ML clearly exhibit an energy gap at $E_F$, which indicates the MIT at a critical film thickness of 2–3 ML. The evolution of the spectral weight at $E_F$ across MIT is more clearly exhibited in Fig. 2(b), the peak position of the incoherent part remains unchanged in all film thicknesses, indicating that $U$ does not change as a function of the film thickness. This means that the MIT in SVO ultrathin films originates from the reduction of bandwidth $W$. The reduction of $W$ with decreasing film thickness is naturally explained by the decrease in the effective coordination number of ions due to the lack of neighboring V ions at the interface and surface. $W$ is scaled with $t$ as $W \sim 2Nm$ ($W \sim 8t$ in 2D and $12t$ in 3D, respectively) in the Hubbard model, where $N$ is the coordination number and $t$ characterizes the energy scale of electron hopping between nearest-neighbor sites. The conduction electrons in SVO are confined in the in-plane direction.

![Figure 2](image2.png)

Figure 2. Schematic illustration for explaining the dimensional-crossover-induced metal-insulator transition in SrVO₃ thin films.

The observed thickness-dependent MIT may be explained in terms of dimensional crossover, as illustrated in Fig. 2. As shown in Fig. 1(b), the peak position of the incoherent part remains unchanged in all film thicknesses, indicating that $U$ does not change as a function of the film thickness. This means that the MIT in SVO ultrathin films originates from the reduction of bandwidth $W$. The reduction of $W$ with decreasing film thickness is naturally explained by the decrease in the effective coordination number of ions due to the lack of neighboring V ions at the interface and surface. $W$ is scaled with $t$ as $W \sim 2Nm$ ($W \sim 8t$ in 2D and $12t$ in 3D, respectively) in the Hubbard model, where $N$ is the coordination number and $t$ characterizes the energy scale of electron hopping between nearest-neighbor sites. The conduction electrons in SVO are confined in the in-plane direction.

**REFERENCES**


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