Self-Energy and the Electronic Structure of Correlated Metal $SrVO_3$

The correlated electronic structure of $SrVO_3$ has been investigated by angle-resolved photoemission spectroscopy (ARPES) using *in situ* prepared thin films. Pronounced features of band renormalization have been observed as in the high-T_c cuprates, such as a sharp kink ~60 meV below the Fermi level (E_F). We have deduced the electron self-energy, which represents the interaction in a solid, in a wide energy range by applying the Kramers-Kronig relation to the photoemission spectra. The obtained self-energy indicates a large energy scale of ~0.7 eV, which is attributed to electron-electron interaction and gives rise to the incoherent peak ~1.5 eV below E_F. The present analysis enables us to obtain a consistent picture for both the high-energy incoherent state and the low-energy band renormalization.

The effect of many-body interaction on the electronic structure, such as electron correlation or electron-phonon interactions, is an important concept for understanding the physical properties of materials. In a correlated electron system, coupling of single-particle excitations with collective excitations such as phonons, leads to a pronounced energy-dependent band renormalization, a so-called kink, in the band dispersion. In the high-T_c cuprate superconductors, a kink has been observed around 60 meV below E_F [1] by angle-resolved photoemission spectroscopy (ARPES) and the origin of the kink has been under debate for a long time. Studies of kinks in transition-metal oxides other than the cuprates would give useful information.

$SrVO_3$ (SVO) is a perovskite-type transition-metal oxide (TMO) and is a prototypical Mott-Hubbard-type system with the d^1 electronic configuration. Therefore, SVO is an ideal system to study the fundamental physics of electron correlation and has been extensively studied by photoemission spectroscopy measurements. Recently, quasi-particle (QP) bands of SVO have been clearly observed by ARPES with the aid of the high-quality films having atomically flat surfaces grown by the pulsed laser deposition (PLD) technique [2, 3]. Here, we present an ARPES study of SVO epitaxial thin films and reveal a kink in the QP band dispersion as well as the self-energy in a wide energy range [4].

The chemical composition of SVO thin films was checked by core-level photoemission spectra measured at BL-2C and the ARPES measurements were performed at BL-28A. Correlation effects in the QP spectra were closely examined for the nearly two-dimensional d_{xy} band. An image plot of the d_{xy} band in energy-momentum space is shown in Fig. 1. There are two main features near E_F: the coherent part (the sharp QP peak within ~0.5 eV of E_F) and the broad incoherent part (often regarded as the remnant of the lower Hubbard band centered ~1.5 eV below E_F). As shown in Fig. 2(a), a kink is seen at around 60 meV below E_F very similar to those observed in the high-T_c cuprate superconductors. The kink in the high-T_c cuprates was associated with the oxygen half-breathing phonon mode of 60 meV by Lanzara *et al.* [1], while antiferromagnetic fluctuations and/or the magnetic resonance mode [5] have also been proposed as possible origins of the kink. Since SVO, unlike the cuprates, does not have low-energy spin fluctuations, the kink observed in the present study is likely due to a coupling of electrons with these phonon modes characteristic to the perovskite oxides.

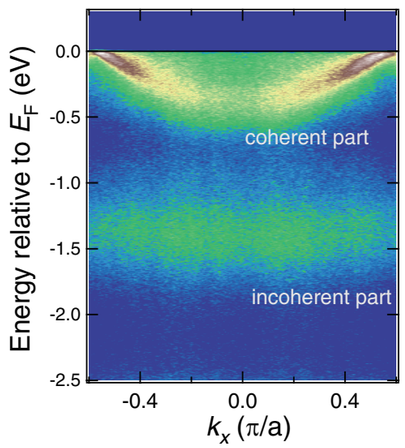

Figure 1: ARPES spectra of SrVO3 along the kx direction taken at the photon energy of 66 eV with linear polarization. The clear band dispersion near EF is the dxy band.

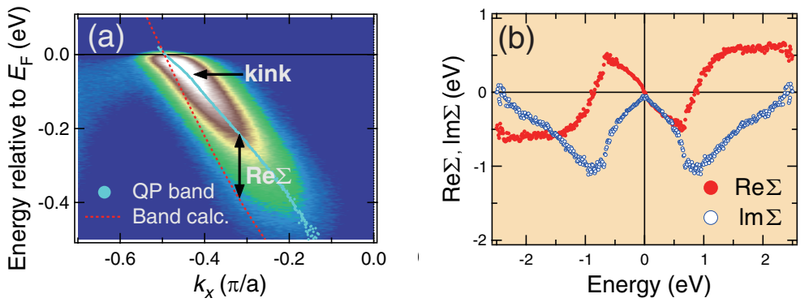

Figure 2: Band dispersions and self-energies in the vicinity of the Fermi level. (a) QP band dispersions are determined by the peak positions (blue dots). The position of the kink at 60 meV is shown by an arrow. The noninteracting band given by the band-structure calculation is shown by red curves. The real part of the self-energy ReΣ can be obtained as the difference between the QP band dispersion and the noninteracting band dispersion. (b) Self-energy deduced from the measured ARPES spectra using the KK transformation.

Not only the kink in the low energy scale, but also the high-energy incoherent structure has been examined by deducing the self-energy $\Sigma(\omega)$ in the high energy region. In the conventional method, the real part of the self-energy ReΣ can be obtained as the difference between the QP band dispersion and the noninteracting band dispersion as described in Fig. 2(a). However, the obtained self-energy $\Sigma(\omega)$ is limited to ~0.5 eV below E_F, which is the energy range of the coherent part, while the behavior of the self-energy over a wider energy range including the incoherent part needs to be clarified to understand the role of electron correlation. Therefore, we have developed a new method to deduce the self-energy in a wider energy range using the Kramers-Kronig (KK) relation [4].

Figure 2(b) shows the experimentally deduced self-energy $\mathrm{Re}\Sigma(\omega)$ and $\mathrm{Im}\Sigma(\omega)$ using the KK relation. The deduced self-energy shows remarkably similar behavior to the self-energy calculated for SVO by the dynamical-mean-field-theory method [6]. The self-energy $\mathrm{Re}\Sigma(\omega)$ shows a large energy scale of 0.7 eV reflecting electron-electron interaction and giving rise to the incoherent peak 1.5 eV below E_F. The present result provides a self-consistent procedure to experimentally deduce the self-energy in correlated electron systems; this procedure will be useful for future studies of strongly electron correlated systems such as the high-T_c superconductors.

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BEAMLINES

BL-28A and BL-2C

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