

Angle-resolved photoemission spectroscopy, optical conductivity, and soft X-ray Raman spectroscopy of quasi-one-dimensional V_6O_{13}

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Abstract

We study the electronic properties of quasi-one-dimensional V_6O_{13} which exhibits a metal–insulator transition using angle-resolved photoemission spectroscopy (ARPES), optical conductivity, and soft X-ray Raman spectroscopy (SXRS). From ARPES, we observe an energy gap of 0.2 eV across the metal–insulator transition with change in the lower Hubbard band. Band dispersion is found only along the b -axis, consistent with highly anisotropic behavior observed in optical conductivity and SXRS measured on the same samples. These results indicate the electronic properties of V_6O_{13} are dominated by b -axis electronic structure. © 2002 Elsevier Science B.V. All rights reserved.

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V_6O_{13} is one of the vanadium oxides taking the mixed valences of $2V^{4+}$ (d^1) and V^{5+} (d^0). Its crystal structure, known as a monoclinic system, has a characteristic structure which includes two types of zig-zag chains running along the b -axis with mono V^{4+} and with mixed V^{4+} and V^{5+} [1]. This compound exhibits paramagnetic metal to paramagnetic insulator transition at $T_I \simeq 150$ K with structural distortion and an antiferromagnetic order at $T_N \simeq 55$ K [2]. The electrical resistivity measured along the a -, b - and c -axis of monoclinic structure show anisotropic behavior with change of order more than 10^4 at $\simeq 150$ K along each direction [3]. The conductivity for both phases is the largest in the b -axis.

In this paper, we report the results of angle-resolved photoemission spectroscopy (ARPES), optical conduc-

tivity, and soft X-ray Raman spectroscopy (SXRS) in mixed valence oxides V_6O_{13} .

The ARPES measurements were carried out on a photoemission spectrometer built at ISSP, using a monochromatic He I source (GAMMADATA). The energy and angular resolutions were set to 15 meV and $\pm 1^\circ$, respectively. V_6O_{13} samples were cleaved *in situ* parallel to the ab -plane and all spectra were recorded within 30 min after cleaving. The sample temperature is 170 K in the metallic phase and 130 K in the insulating phase. The Fermi level (E_F) of V_6O_{13} was referenced to that of a gold film. The SXRS measurements were carried out at BL-2C, the Photon Factory. The single crystal growth and sample characterization are described elsewhere [3].

Fig. 1 shows the “band dispersion” near E_F of V_6O_{13} obtained from ARPES spectra taken the second derivative after moderate smoothing, and plotted the intensity as a function of the wave vector and the binding energy. We compare the band structures of the a -axis and the b -axis in the metallic phase [Fig. 1(a) and

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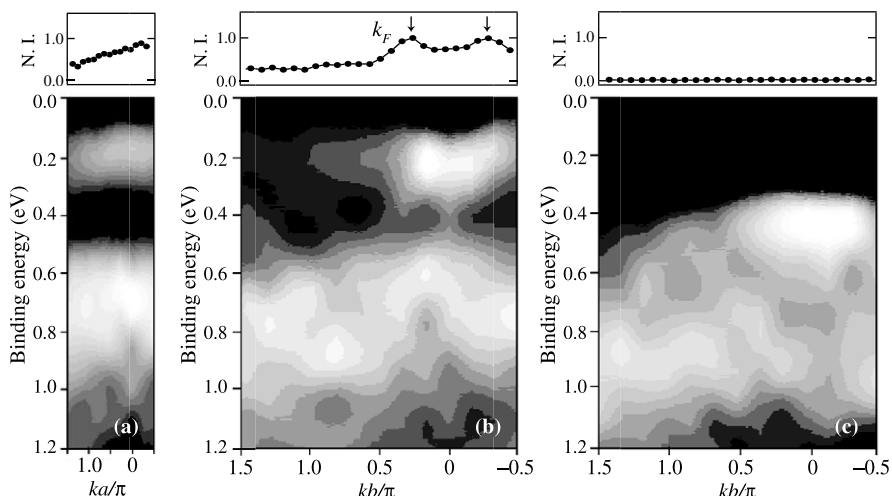


Fig. 1. Second derivative intensity maps near E_F of V_6O_{13} obtained from ARPES spectra measured along (a) a -axis at 170 K, (b) b -axis at 170 K, and (c) b -axis at 130 K. Light areas indicate “bands”. Upper panels show MDCs at E_F .

(b)]. In both directions, we observe mainly two bands; the broad band at 0.8 eV, which may be corresponding to the lower Hubbard band, and the narrower band at about 0.2 eV. While the two bands along the a -axis have almost no dispersion within the first Brillouin zone, those along the b -axis are found to have clear dispersion. Especially, the band at 0.2 eV along the b -axis seems to have upward dispersion tending towards E_F , and shows E_F crossings as determined by two peaks in the momentum distribution curve (MDC) at E_F , though the intensity near E_F is strongly reduced. These results can be attributed to the quasi-one-dimensionality expected from the crystal structure with the zig-zag vanadium chains running along the b -axis. On the other hand, the MDC below T_t has a smaller intensity with no peak structure, which results from opening of an energy gap of 0.2 eV (spectra are not shown here). These observations indicate the change in the electronic structures across the metal–insulator transition. In addition, we observe that the lower Hubbard band slightly shifts to higher binding energy with the 0.2 eV band in the high temperature phase becoming a shoulder structure [Fig. 1 (c)].

Fig. 2 shows: (a) optical conductivity obtained by a Kramers–Kronig transform of the reflectivity spectra and (b) SXRS spectra measured at 298 K along the a - and b -axis. Each result exhibits highly anisotropic behavior. In both measurements, the spectral weight around low energy region along the b -axis is stronger than that along the a -axis. Such response indicates large contribution of the conductive electron near E_F . These anisotropic behavior support the ARPES results indicating the

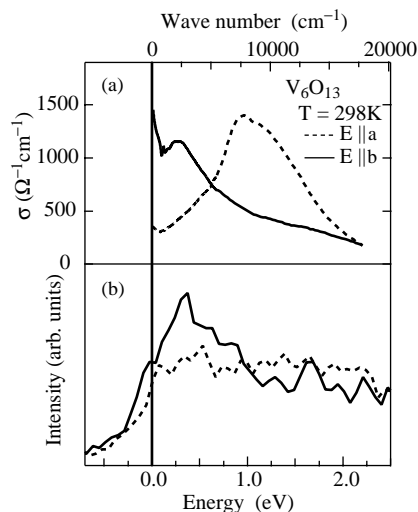


Fig. 2. (a) Optical conductivity and (b) SXRS spectra measured for $E_{\parallel}a$ (dotted line) and $E_{\parallel}b$ (solid line) at 298 K.

quasi-one-dimensional electronic structure along the b -axis.

In conclusion, we have investigated the electronic properties of V_6O_{13} using ARPES, optical conductivity, and SXRS. We observe an energy gap of 0.2 eV across the metal–insulator transition in ARPES. Band dispersion is found only along the b -axis, consistent with highly anisotropic behavior observed in optical conductivity and SXRS. These results indicate the electronic properties of V_6O_{13} are dominated by the b -axis electronic structure.

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