Fermi Surfaces and Kink in the Energy Dispersions of Sr_2RuO_4

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The sudden change of the group velocity, so-called the "kink", of the dispersing peak in angle-resolved photoemission spectroscopy (ARPES) spectra is widely reported in the high-temperature superconducting cuprates. Nevertheless, the interpretations of the kink for the cuprates have been controversial. In previous works, electronic coupling to a bosonic mode such as phonons or magnetic excitations has been discussed as the origin. Recently, we have found a similar kink in the dispersion of the layered perovskite strontium ruthenates [1]. This means that the kink is not peculiar to the cuprates. The layered strontium ruthenates with perovskite-based crystal structure are isostructural to the cuprates, while the electronic and magnetic properties are quite different. The electronic structure close to the Fermi level (E_F) of the layered ruthenates is derived not only from the in-plane Ru $4d_{xy}$-O $2p$ band but also from the out-of-plane Ru $4d_{yz,zx}$-O $2p$ ones, while for the cuprates a single in-plane Cu $3d_{x^2-y^2}$-O $2p$ band plays a crucial role. Therefore, ARPES study on the layered ruthenates is expected to provide insight into the origin of the kink in transition metal oxides.

The electronic bands near E_F are derived mainly from the Ru t_{2g} orbitals; the band due to the in-plane Ru $4d_{xy}$ orbital exhibits two-dimensional character with a large energy dispersion, while the bands due to the out-of-plane Ru $4d_{yz}$ and $4d_{zx}$ orbitals exhibit nearly one-dimensional character with a small energy dispersion. Previous ARPES and de Haas-van Alphen (dHvA) studies showed the Fermi surface (FS) exhibiting one hole sheet (α) and two electron sheets (β and γ), qualitatively consistent with the LDA calculation. The α and β sheets are derived from the out-of-plane Ru $4d_{yz}$ and $4d_{zx}$ orbitals, while the remaining γ sheet is from the in-plane Ru $4d_{xy}$ orbital. Here, we present detailed band dispersion and FS's of Sr_2RuO_4, determined by high-resolution ARPES, to elucidate the orbital selectivity of the kink. A kink in the dispersion is clearly shown for this *xy* band, while not for the *yz, zx* ones.

In order to obtain clean surfaces without the replica of FS's in the bulk due to the surface rotation, we cleaved the single crystalline Sr_2RuO_4 samples *in situ* in ultrahigh vacuum (below 1×10^{-10} Torr) at 160K. The spectral weight due to the surface state at the (π,0) point was almost eliminated, and the coherent peak dispersion and line shape are qualitatively consistent with the dHvA measurements and the LDA band predictions. The present measurements were carried out at a new high-resolution and high-flux undulator beamline (BL-28) of the Photon Factory (KEK, Tsukuba). The sample goniometer used here provides independent polar and tilt rotations of the sample (R-Dec Co. Ltd., *i* GONIO LT) [2]. The beamline is equipped with a high-resolution, hemispherical electron analyzer (Gammadata-Scienta SES-2002). The emission angle of the photoelectron with respect to the surface normal was varied by rotating the polar and tilt axes of the sample.

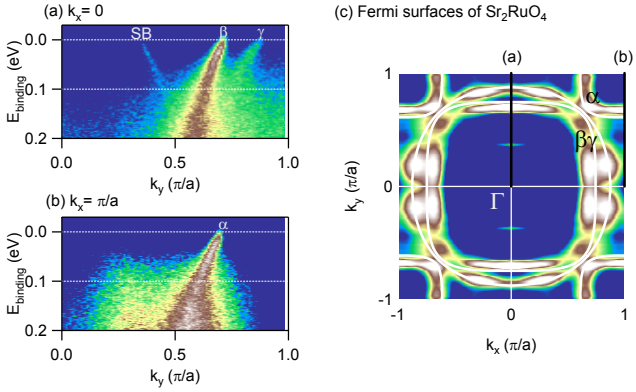

FIG. 1: (a) and (b) Intensity plots along (0,0)-(0,π) and (π,0)-(π,π), respectively. (c) E_F intensity map. The white lines means the Fermi surface based on the LDA calculation.

Figure 1 (a) and (b) show the Intensity plots along (0,0)-(0,π) and (π,0)-(π, respectively. A kink in the dispersion is shown for the γ band, while not for the α and β bands. The Fermi surfaces (Fig. 1 (c)) are qualitatively consistent with the LDA band prediction (wihte lines). Here, we will discuss the origin of the kink of Sr_2RuO_4.

[1] Y. Aiura *et al.*, Phys. Rev. Lett. **93**, 117005 (2004).
[2] Y. Aiura *et al.*, Rev. Sci. Instrum. **74**, 3177 (2003).