High-resolution angle-resolved photoemission study of Fe (110)

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Abstract

High-resolution low-temperature angle-resolved photoemission spectroscopy of Fe(110) single crystal has been done to evaluate many-body interactions on the quasi-particles at the Fermi level. A kink structure in the minority-spin band ($B_{\downarrow}$) on the Fermi surface (FS) around the Γ point has been clearly observed at the binding energy of ~40 meV, but it is absent for the majority-spin band ($B_{\uparrow}$) on the FS around the Γ point. Additional spectral feature has been observed for $B_{\uparrow}$, indicating a coexistence of a surface resonance state. By the analyses of the imaginary part of the self-energy, we have confirmed that the kink structure is derived from the electron-phonon interaction.

Keywords: angle-resolved photoemission spectroscopy, Fe(110), surface resonance state, self-energy

The electronic structure of ferromagnetic bcc iron has been studied extensively so far theoretically and experimentally [1-3]. However, direct examination of the self-energy derived from many-body interactions has not been directly clarified yet. Owing to recent development of high energy- and angular-resolutions of angle-resolved photoemission spectroscopy (ARPES), now we can experimentally estimate the energy and momentum dependence of the self-energy.

In the present paper, we report high-resolution ARPES measurements on Fe(110) single crystal at low temperature. By means of quantitative analyses of the spectral shape, we will examine many-body interactions of quasi-particles at the Fermi level (E_F).

ARPES measurements were done on the linear undulator beamline BL-1 of a compact electron-storage ring (HiSOR) at Hiroshima Synchrotron Radiation Center (HSRC), Hiroshima University [4]. The Fe(110) single crystal sample was cleaned by repeated cycles of Ar^+ bombardment and subsequent annealing at 570 ℃ [3]. Cleanliness of the sample surface was checked by Auger electron spectroscopy. We set photon energy at hν=78.9 eV and temperature at 10 K. Energy and angular resolutions were set at ΔE=20 meV and Δθ=0.3 degree, respectively. We examined energy bands on the minority-spin and majority-spin Fermi surfaces (FSs) around the Γ point.

Figs. 1(c) and 1(d) show the intensity plots of the minority-spin and majority-spin bands, respectively. Here we denote these bands as $B_{\downarrow}$ and $B_{\uparrow}$. As the momentum distribution curve (MDC) at E_F in Fig. 1(b) shows, the $B_{\uparrow}$ band is accompanied by a weak structure denoted here as S. According to the band-structure calculation, only one bulk-derived majority-spin band is predicted [1]. We interpret the S band in terms of the surface resonance state, which overlaps energetically with the bulk derived band [5,6].

The peak positions [dots in Figs. 1(c) and (d)] were obtained by fitting MDCs with Lorentzians on linear background. We should note that in Fig. 1(c) the $B_{\downarrow}$

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band dispersion exhibits a "kink structure", or a sudden change of the group velocity, at ~40 meV. Since the Debye temperature of Fe is Θ_D =470 K ($k_B\Theta_D$ =40.4 meV), it is reasonable to assume that this kink structure is derived from the electron-phonon interaction.

The imaginary part of self-energy (ImΣ) can be directly evaluated by the photoemission spectral width (δE) along the energy direction, 2|ImΣ| = δE. We evaluated δE using a formula, $\delta E = (dE/dk)\delta k$, where dE/dk is the gradient of the energy-band dispersion, δk the MDC width [7].

In Fig. 1(e), 2|ImΣ| of the B$\downarrow$ band shows a pronounced decrease below ~40 meV, which coincides with the energy scale of the kink structure and the Debye temperature. It clearly indicates that the kink structure is not derived from the energy-band dispersion, but from the many-body interaction, namely, the electron-phonon interaction. On the other hand, one cannot see a decrease at ~40 meV in 2|ImΣ| of the B$\uparrow$ and S bands, in agreement with the absence of the kink structure. This result clearly indicates that the magnitudes of the electron-phonon coupling for the FSs around the Γ point are different depending on the spin direction.

On the basis of the Fermi-liquid theory [7], 2|ImΣ| should be in proportion to ω^2 near E_F at low temperature. Solid curves in Figs. 1(e) and 1(f) represent fits of observed 2|ImΣ|. The energy dependence of 2|ImΣ| for B$\uparrow$ and S bands are well explained by the Fermi-liquid theory. For the B$\downarrow$ band, we can see a good agreement for the deeper binding energy side (E_B>~40 meV).

In summary, high-resolution low-temperature ARPES of Fe(110) single crystal has been performed. A kink structure at ~40 meV has been observed for the B$\downarrow$ band but it is absent for the B$\uparrow$ band. We found a surface resonance state for the B$\uparrow$ band. On the basis of the energy dependence of the self-energy, the kink structure in the B$\downarrow$ band should be derived from the electron-phonon interaction. The magnitudes of the electron-phonon interaction for the FSs around the Γ point are different depending on the spin direction.

The experiments have been conducted under the approval of HSRC (Proposal No. A05-12). This work was partly supported by a Grant-in-Aid (Grant No. 17654060) from MEXT of Japan.

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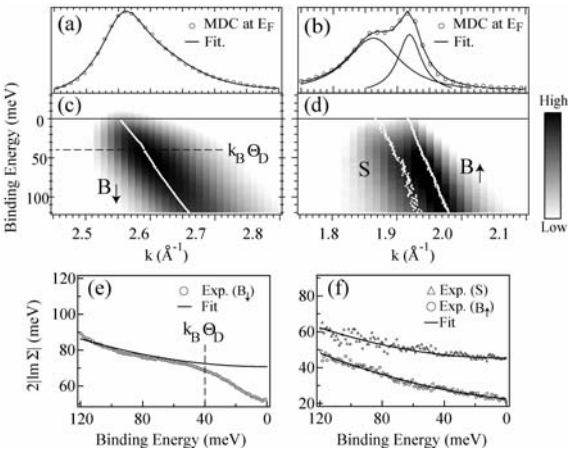

Fig. 1. ARPES results of Fe(110) with hν = 78.9 eV at 10 K. (a) and (b) exhibit MDCs at E_F for B$\downarrow$ and B$\uparrow$, respectively. (c) and (d) show intensity plots of B$\downarrow$ and B$\uparrow$, respectively. (e) and (f) indicate experimentally evaluated 2|ImΣ| for B$\downarrow$ and B$\uparrow$, respectively. White dots in (c) and (d) indicate evaluated peaks locations. Solid lines in (e) and (f) show fits assuming ω^2-dependence.