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↓) 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↑) on the FS around the Γ point. Additional spectral feature has been observed for B↑, 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 °C [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↓ and B↑. As the momentum distribution curve (MDC) at E_F in Fig. 1(b) shows, the B↑ 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↓
band dispersion exhibits a "kink structure", or a sudden change of the group velocity, at \( \sim 40 \) meV. Since the Debye temperature of Fe is \( \Theta_D = 470 \) K (\( k_B \Theta_D \approx 40.4 \) meV), it is reasonable to assume that this kink structure is derived from the electron-phonon interaction.

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

In Fig. 1(e), \( 2|\text{Im}\Sigma| \) of the \( B_\downarrow \) band shows a pronounced decrease below \( \sim 40 \) 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 \( \sim 40 \) meV in \( 2|\text{Im}\Sigma| \) 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 \( \Gamma \) point are different depending on the spin direction.

On the basis of the Fermi-liquid theory [7], \( 2|\text{Im}\Sigma| \) should be in proportion to \( \omega^2 \) near \( E_F \) at low temperature. Solid curves in Figs. 1(e) and 1(f) represent fits of observed \( 2|\text{Im}\Sigma| \). The energy dependence of \( 2|\text{Im}\Sigma| \) 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 (\( E_B > \sim 40 \) meV).

In summary, high-resolution low-temperature ARPES of Fe(110) single crystal has been performed. A kink structure at \( \sim 40 \) 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 \( \Gamma \) point are different depending on the spin direction.

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References
[6] In our unpublished data, the S band disappears quickly by oxygen absorption, supporting our interpretation.