

The Fermi surface and sheet-dependent superconducting gap of MgB_2

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Abstract

The Fermi surface and superconducting gap of MgB_2 have been studied by angle-resolved photoemission spectroscopy. Two Fermi surfaces composed of the σ band and the π band are clearly observed without contaminated by the “surface-derived” band. The high-resolution photoemission spectra show that superconducting gaps with values of 5.5 and 2.2 meV open on the σ band and the π band, respectively, both of which close at the bulk transition temperature (T_c). This result provides an experimental evidence for the two-band superconductivity on MgB_2 and, moreover, validates the role of momentum-dependent electron–phonon coupling as the origin of multiple-gap superconductivity as well as the high transition temperature (T_c) of MgB_2 .

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1. Introduction

After the discovery of unexpectedly high transition temperature (T_c) of MgB_2 [1], many studies have been done to understand the superconducting (SC) transition mechanism. The isotope effect on

T_c strongly suggests the phonon-mediated superconductivity [2]. Likewise the multiple SC gap is observed from specific heat, tunneling spectroscopy, Raman spectroscopy [3], angle-integrated photoemission (AIPE) spectroscopy [4], and so on [5]. Being one of the most outstanding features in the electronic structures of MgB_2 , the multiple gap has been thought to be a clue to the mechanism producing the high T_c . The first-principles calculations [6,7] predict that MgB_2 has two kinds of electronic bands. One is two-dimensional (2D)

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band derived from the σ orbital of boron 2p (namely σ band) and the other is three-dimensional (3D) one derived from the π orbital (namely π band). Theoretical works also [8,9] suggest that the electron–phonon coupling strength depends on the dimensionality; the σ band couples to in-plane phonon mode stronger than the π band does, and this difference leads to the multiple gap. Though there is much experimental evidence of the multiple gap as mentioned above, those are indirect and, at least partially, give momentum (k)-integrated information.

On the other hand, the angle-resolved (AR) photoemission (PE) spectroscopy is the best ways to study the k -dependent electric states including a SC gap. The previous works [10,11] show the bulk band dispersions together with a so-called surface band. Unfortunately the k -position where the σ band crosses the Fermi level (E_F) are hindered by that of the surface-derived band with much more pronounced intensities. In such condition, it may be hard to distinguish the superconducting gap of the σ band from that of the surface band, as they showed similar gap values [10]. Due to the presence of the surface derived bands, there is no ARPE report for FSs of MgB_2 .

In this paper, extending our recent study [12], we present first experimentally obtained FS using ARPES, σ and π band dispersions clearly isolated from the surface band, and Fermi-sheet dependent SC gap. These results reveal the nature of the multiple SC gap of MgB_2 .

2. Experimental

The MgB_2 single crystals for this ARPE study were synthesized under high pressure and high temperature. The detail is described elsewhere [13]. The superconducting transition at about 36 K was confirmed from magnetization measurements [13]. The instrumental details were described in another paper [12]. All the ARPE spectra in this work were obtained using $\text{HeII}\alpha$ (40.814 eV) resonance line. The energy and angular resolutions for the wide-range valence band measurements were set to ~ 100 meV and $\pm 0.1^\circ$, respectively. The high-resolution measurements for SC gap on the σ band

and π band were set to energy resolution 5.0 and 3.9 meV, respectively, depending on the count rate.

3. Results and discussion

Fig. 1 shows the ARPE intensity map as a function of (a) k_x and k_y (b) k and a binding energy (BE), where the black area indicates higher intensity. The intersection of the FSs with the $k_z = 0$ plane is shown in Fig. 1(a), where two small (thin solid lines) and one large (thin broken line) circular sheets correspond to the 2D FS sheets and one of the 3D sheet, respectively. Lower hexagon corresponds to the first Brillouin zone (BZ). The gray scale pattern in Fig. 1(a) was obtained by summing up the photoemission intensity over ± 50 meV of E_F and higher intensity region indicates the FSs. To emphasize the structure, the intensity around the $\Gamma(A)$ point in the second BZ is multiplied by a factor of 3. Mainly two higher intensity regions are observed. One is prominent arc around the $M(L)$ point and this can be assigned to the π band from a comparison with the calculation [7]. The other is circular centered at the $\Gamma(A)$ point of the second BZ, which can be assigned to the FS of the σ band, too. No other prominent area had been observed including around the $\Gamma(A)$ point of first BZ, where it is expected to observe two FSs of the σ band and one FS of the surface band.

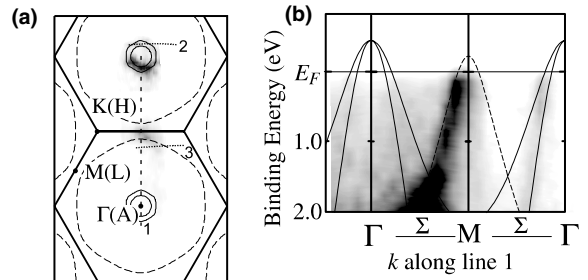


Fig. 1. Photoemission intensity map (a) at the Fermi level as a function of k and (b) along $\Gamma(A) - M(L) - \Gamma(A)$ line as a function of the binding energy and k . The calculated Fermi surface and band dispersion on $k_z = 0$ plane are superimposed by the thin solid lines for the σ band and the thin broken lines for the π band. Those are in agreement with each other. The slight discrepancy of the k position can be explained supposing the $k_z \neq 0$ plane is observed (see text).

Fig. 1(b) shows an intensity map of ARPES spectra measured along the $\Gamma(A) - M(L) - \Gamma(A)$ high symmetry line (line 1 in Fig. 1(a)), compared with the calculated band dispersions on the $k_z = 0$ plane (thin solid lines for the σ band and thin broken lines for the π band). One can clearly see a prominent feature that disperses toward E_F in the first BZ. Having an agreement with the calculated π band in terms of the dispersion, this band can be ascribed to the π band. The observation of the π band in the $k_z = 0$ plane suggests that the measured k_z position with the photon energy we used is located near the $k_z = 0$ plane. Besides the prominent structure, we also find another dispersive feature that crosses E_F near the $\Gamma(A)$ point in the second BZ. It is found that this band follows the dispersion of one of, closer to $\Gamma(A)$ point, the calculated σ bands and therefore can be assigned to the inner σ band. Both the experimental σ band and π band are slightly different from the calculated ones in terms of k point similarly to FS case. This means that the spectra is obtained on the $k_z \neq 0$ because the k_F of the σ band and π band will shift to $M(L)$ point direction with deviating from $k_z = 0$, as expected from band calculation [9].

The previous ARPES measurements [10,11] in the first BZ observed σ band and π band with an additional so-called surface band. In the present study, we found no clear evidence for the surface band in the first and second BZ. Inability to observe the π band in the second BZ and the other σ band in the second BZ can be also attributed to matrix element effects, which strongly affects the intensity of photoelectrons as has been demonstrated for single crystal graphite [14].

Thus, the identification of σ and π band derived FS sheets provides us the opportunity to measure the SC gap independently on each FS sheet without the surface contribution. Fig. 2(a) and (b) show temperature-dependent high-resolution ARPES spectra near E_F obtained along lines 2 and 3 in Fig. 1(a), respectively. Here we employ higher resolution (5.0 meV for the σ band and 3.9 meV for the π band). To make up for the very low count rate when using higher resolution and due to the small sample size, the spectra shown are the sum of the APRE spectra obtained along lines 2 and 3, and, thus, correspond to partially angle-integrated

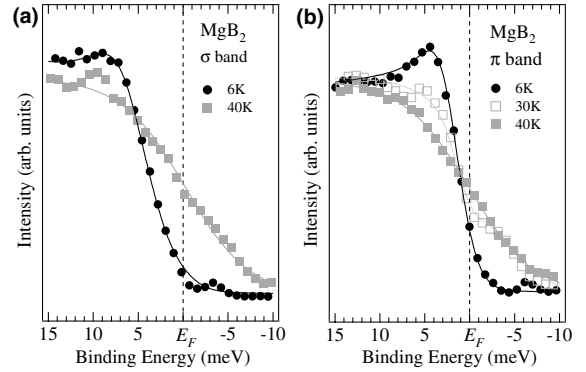


Fig. 2. High-resolution and temperature-dependent photoemission spectra of (a) σ band and (b) π band. The spectra obtained at 6 K show the mid-point shift of the spectral edge for 3.6 meV for the σ band and 0.9 meV for the π band indicating the opening of the different magnitudes of superconducting gaps for each band. The fitting result using a Dynes function is superimposed with lines.

spectra but for each individual band. This justifies the use of the modified BCS function, known as a Dynes function, analysis for angle-integrated spectra [15]. At 6 K, the spectrum of the σ band has a broad peak around 10 meV and a leading-edge shift of 3.6 meV. The leading-edge shift of a SC spectrum has been used to qualitatively estimate the size of a SC gap. The spectrum measured at 6 K on the π band has a more pronounced condensation peak but shows a leading-edge shift of only 0.9 meV. The larger shift on the σ band than on the π band in spite of the lower resolution used for the σ band strongly indicates that sizes of the SC gap are highly dependent on the character of the bands. The small shoulder structure near E_F of 30 K spectra of the π band is indicative of persistence of the SC gap close to the bulk T_c of 36 K, indicating that the smaller gap on the π band originates in the bulk electronic structure, too. Therefore, we can conclude that these raw data themselves provide definitive experimental evidence for the two-band superconductivity of MgB_2 .

For a more quantitative discussion, we estimated the size of the gap using a Dynes function, which includes the magnitude of a SC gap Δ and the quasiparticle lifetime broadening Γ [16]. The results are superimposed as lines shown in the

Fig. 2(a) and (b). It can be seen that the function well reproduces the raw spectra. The size of the SC gap for the σ and π bands are plotted as a function of temperature with open circles and diamonds in Fig. 3, respectively, together with that expected from conventional BCS theory [16] for two gaps (lines). The π band gap almost completely obeys the BCS temperature dependence and the σ band gap is slightly smaller than the theoretical one. This result is qualitatively consistent with theoretical prediction [8]. As was implied by the raw data, the smaller gap of the π band persists up to the bulk T_c , further confirming the bulk origin. At the lowest temperature within our measurements, the gap values are 5.5 meV for the σ band and 2.2 meV for the π band. Correspondingly, the reduced gap parameter $2\Delta/k_B T_c$, where k_B is the Boltzmann's constant, is 3.54 for the σ band and 1.42 for the π band, indicating weak coupling of π . The present σ - and π -band SC-gap values agree well with the previous angle-integrated (AI) PES [4] with a slightly smaller value for the gap on the π band in ARPES compared to that of the smaller gap in AIPES, including the temperature dependence of the gap values. The consistent values

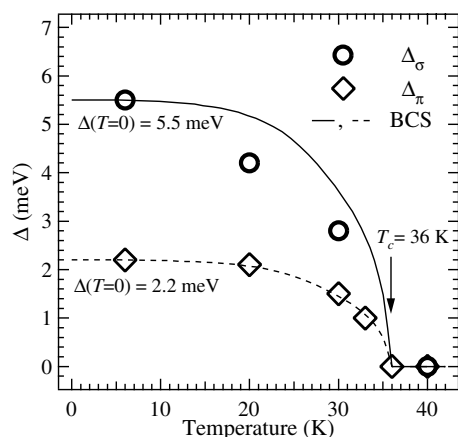


Fig. 3. Temperature dependence of the superconducting gap. The open circles and diamonds indicate the experimentally decided temperature dependence of the gap. The temperature dependence of the gap expected from BCS theory [16] is superimposed by the solid line for the σ band and the broken line for π band, respectively. The values of $\Delta(T = 0 \text{ K})$ for each band were determined from the experimental values 5.5 meV for s band and 2.2 meV for p band obtained at 6 K and the T_c was set to 36 K.

obtained with ARPES and AIPES for the gap on the π band suggests that the anisotropy of the SC gap on the π band is very small.

The present ARPES studies identify the larger gap on the σ band and the smaller gap on the π band and thus provide direct experimental evidence for the two-band superconductivity in MgB_2 . The present results also emphasize the importance of a FS sheet-dependent gap. The experimental confirmation of the two-band superconductivity predicted by the first-principles band calculations dealing with k -dependent electron–phonon coupling [8,9], in turn, confirms the importance of the k -dependent electron–phonon coupling to the SC properties of MgB_2 , including the high T_c .

In conclusion, we have performed high-resolution ARPE measurements of MgB_2 in order to study the origin of the multiple gap reported from k -integrated experimental probes and obtained the information of the FS, the valence band dispersion, and the superconducting gap. The FS and valence band spectra show the surface-free σ band. The high-resolution spectra show the magnitude of the gap to be 5.5 and 2.2 meV at 6 K for the σ and π bands, respectively, and simultaneous gap closure at the bulk T_c . This provides direct experimental evidence for the two-band superconductivity of MgB_2 . The experimental observation of the two-band superconductivity predicted by first-principles band calculations with k -dependent electron–phonon coupling confirms the importance of k -dependent electron–phonon coupling [8,9] for the SC properties of MgB_2 , including the high T_c .

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