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Review

Recent photoemission studies on MgB_2 and related materials

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Abstract

MgB_2 shows the highest superconducting transition temperature among intermetallic compounds. Angle-resolved photoemission spectroscopy revealed their electronic structure, and the result is well explained within a simple band picture except for one band. Other photoemission studies on related materials of AlB_2 and CaAlSi also show an extra band similar to that in MgB_2. The direct observation of the superconducting gap confirmed a two-gap superconductivity. The larger and smaller gaps open at the σ and π bands, respectively. The carbon substitution effect on the two gaps was evaluated by using sub-meV photoemission spectroscopy.

Keywords: Photoemission spectroscopy; Band structure; Superconducting gap

Contents

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1. Introduction

A recent instrumental development in photoemission spectroscopy (PES) offers us a unique opportunity to observe the detailed electronic structure because PES reflects the occupied electronic state. In particular, angle-resolved PES (ARPES) yields the energy and momentum resolved electronic structure. The combination of ARPES and high energy resolution directly reveals the gap anisotropy, which is well known to exist in cuprate superconductors [1].

Earlier, a large number of studies were reported [2] soon after the discovery of the superconductivity of MgB_2 [3] due to its high superconducting (SC) transition temperature (T_c) of 39 K, which is close to or even higher than the BCS limit. Nowadays, the SC mechanism of MgB_2 is understood within the electron–phonon scenario [4,5]. To achieve such a high T_c, strong electron–phonon interaction is essential. In fact, Raman spectroscopy [6,7] and inelastic X-ray scattering spectroscopy [8] provide experimental evidence for this strong coupling. These facts reinforce the electron–phonon scenario.

The outstanding feature of MgB_2 is not only the T_c but also a multiple SC gap. Since its discovery, some experimental studies offered the possibility of a multiple SC gap [2]. However, all of them required some assumptions and/or analyses. Therefore, more concrete evidence is required for a definite conclusion. With regard to this, the APRES is presently considered to be the best method.

In this paper, we review the recent PES results of MgB_2 and related materials to summarize the studies after the prior review [9]. The overall electronic structure and multiple SC gap are definitively clarified. A theoretical analysis suggests the importance of the interband interaction for realizing a higher T_c.

2. ARPES

2.1. Principles

Many readers are already familiar with the principle of PES; therefore, we would like to briefly mention it here. More detailed explanations are provided in many textbooks (see for example [10]).

At present, ARPES is the only practical method to observe energy and momentum at the same time inside the solid directly. The PES process is based on the energy and momentum conservation law. This energy conservation law is represented by Einstein's relation, which is given by the following expression:

$$E_B = h\nu - \phi - E_k,$$

where $h\nu$ is excitation energy; ϕ, the work function; E_B, the binding energy of electron inside the solid; and E_k, the kinetic energy of the photoelectron. By observing E_k, we can directly know E_B. Further, if the sample surface is atomically flat and sufficiently clean, the momentum of the photoelectron can be estimated to obtain the emission angle together with E_k because the momentum parallel to the sample surface is conserved inside and outside the sample. By changing the emission angle and excitation energy, we can map out the full band structure.

PES has some drawbacks. One of them is the energy resolution. Sometimes, PES has a worse energy resolution than other techniques like tunneling spectroscopy. Another drawback is the surface sensitivity. The recent instrumental development in the PES system achieved up to an energy resolution of the sub-meV order [11]. This high energy resolution is suitable for observing the SC gap of even low T_c materials like Pb, $CeRu_2$, etc. [11,12]. Further, instrumental improvement leads to relatively bulk sensitive PES. Very high and very low kinetic photoelectrons interact less with the surrounding ions [13]. In this review, PES is obtained by a high-resolution He discharge lamp (21.218 eV and 40.814 eV), synchrotron radiation (28 eV, 50–90 eV, 875 eV), and the vacuum-ultra-violet (VUV) laser (6.994 eV). Considering the phenomenological universal relation [13], the electron escape depth is estimated to be less than 1 nm for a 20–185 eV excitation, ~1.6 nm for a 875 eV excitation, and ~3 nm for a 7 eV excitation. The PES with 875 eV excitation and VUV laser excitation is relatively bulk sensitive.

2.2. Valence band, Fermi surface, and surface state

Uchiyama et al. confirmed that the overall valence band structure is explained almost completely within the simple first principles calculations, except for one extra band that disperses parabolically around the Γ point [14]. After Uchiyama et al., ARPES studies were reported by Tsuda et al. [15,16], Souma et al. [17,18], and Cepek and Petaccia et al. [21,19]; some of them observed the extra state of MgB_2 by these studies [17,18,21,19].

Fig. 1 shows one of the results [15] and presents the band dispersion of MgB_2 along the Γ–M–Γ line obtained with HeIIα excitation (Fig. 1a). The horizontal and vertical axes correspond to the momentum and binding energy, respectively. The higher intensity area is shaded black. The left and right hand sides are the first and second Brillouin zones, respectively. The calculated band dispersion is superimposed by solid and broken curves corresponding to the σ and π band, respectively [20]. In the first Brillouin zone, a π band is clearly observed while the σ band and surface band are not clear. In the second Brillouin zone, a σ band is clearly observed. These band dispersions agree well with the calculated one.

Fig. 1b shows the intensity map on the k_x–k_y plane at Fermi energy. The thick hexagonal lines represent the border of each Brillouin zone. The solid and broken curves represent the Fermi surface of the σ and π bands, respectively [20]. The two Fermi surfaces are separately observed around the M(L) and Γ(A) points. The shape of the Fermi surface is well reproduced by the first principles calculations [20].