

High-Resolution Photoemission Study of MgB₂

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We have performed high-resolution photoemission spectroscopy on MgB₂ and observed opening of a superconducting gap with a narrow coherent peak. We found that the superconducting gap is *s* like with the gap value (Δ) of 4.5 ± 0.3 meV at 15 K. The temperature dependence (15–40 K) of the gap value follows well the BCS form, suggesting that $2\Delta/k_B T_c$ at $T = 0$ is about 3. No pseudogap behavior is observed in the normal state. The present results strongly suggest that MgB₂ is categorized into a phonon-mediated BCS superconductor in the weak-coupling regime.

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The discovery of noncuprate “high-temperature” superconductor MgB₂ [1] has evoked much attention in how this simple binary superconductor is similar to or different from the “conventional” high-temperature superconductors (HTSCs). The superconducting transition temperature (T_c) exceeds those of known metal superconductors and alkali-doped C₆₀, being comparable to that of one of the HTSCs (La_{2-x}Sr_xCuO₄), and is located just on or a little above the theoretical upper limit predicted for the phonon-mediated superconductivity [2]. It is thus quite important to elucidate the mechanism and origin of this newly discovered “high- T_c ” superconductor in relation to the cuprate HTSCs. The superconducting gap and its symmetry have been investigated by tunneling [3–5] and NMR spectroscopy [6], but the results are not necessarily consistent with each other. Photoemission spectroscopy (PES) has revealed many key physical features of cuprate HTSCs such as the pseudogap [7,8] and quasiparticles [9,10]. A recent remarkable progress in the energy resolution enables direct observation of a superconducting gap in metal superconductors [11,12].

In this Letter, we report high-resolution PES results on MgB₂ to study the superconducting gap and its symmetry. By using a merit of high energy resolution ($\Delta E < 5$ meV), we have succeeded in directly observing opening/closure of the superconducting gap as a function of temperature, together with a narrow superconducting coherent peak located slightly below the Fermi level (E_F). We have performed numerical fittings to the PES spectra to investigate the size and symmetry of the superconducting gap.

The procedure to prepare polycrystalline MgB₂ samples has been described elsewhere [1]. The x-ray diffraction measurement shows that the samples are single phased and the electrical resistivity and dc magnetization measurements confirm a sharp superconducting transition onset at 39.5 K. High-resolution PES measurements were performed using a SCIENTA SES-200 spectrometer with a high-flux discharge lamp and a toroidal grating monochromator. We set the total energy resolution at 4–7 meV to obtain a reasonable count rate near E_F . The base pressure of the spectrometer was 1.5×10^{-11} Torr. Samples

were scraped *in situ* with a diamond file to obtain a clean surface for PES measurements. A measured PES spectrum represents the density of states since the sample is a polycrystal. The temperature of the sample was monitored with a calibrated silicon diode sensor to an accuracy of ± 0.5 K. We have confirmed the results shown here being reproducible for repeated scraping and on a cycle of increasing/decreasing temperature. The Fermi level of the sample was referenced to that of a gold film evaporated onto the sample substrate and its accuracy is estimated to be better than 0.2 meV.

Figure 1 shows PES spectra near E_F of MgB₂ measured with a He I α resonance line (21.218 eV) at temperatures (15 and 50 K) below/above the T_c (39.5 K). The spectral intensity is normalized to the area under the curve. According to the band structure calculations, the electronic states near E_F originate in the *B* 2*p* states [13,14]. As seen

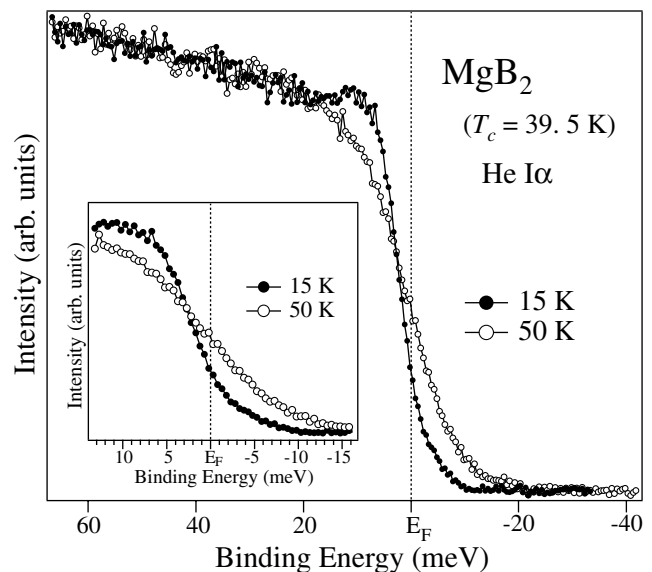


FIG. 1. High-resolution PES spectra near E_F of the MgB₂ polycrystal measured with a He I α resonance line (21.218 eV) at temperatures (15 and 50 K) below/above the T_c (39.5 K). The spectral intensity is normalized to the area under the curve. The inset shows the expansion near E_F .

in Fig. 1, the PES spectrum shows a remarkable temperature dependence which is not accounted for by a simple temperature effect due to the Fermi-Dirac function. The midpoint of the leading edge in the PES spectrum at 15 K is not at E_F , but is shifted by a few meV toward the high binding energy relative to E_F (see the inset of Fig. 1). In contrast, the PES spectrum at 50 K appears to have a leading-edge midpoint at E_F , though the position is not well defined due to the broad feature of the PES spectrum. It is remarked here that the 15 K spectrum has a “peak” structure around 10 meV, which totally disappears at 50 K. A similar peak structure has been observed in cuprate HTSCs such as $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$, where the peak is located at a much higher binding energy (about 40 meV) and is ascribed to the superconducting coherent peak [15]. Thus the present temperature-dependent PES results unambiguously show that a superconducting gap of a few meV opens at E_F in MgB_2 at low temperatures. The observed temperature-induced change of the PES spectrum is understood in terms of a “pileup” of the electronic states transferred from the near- E_F region at the superconducting state.

The next problem to be solved is the size and symmetry of the superconducting gap. Figure 2 shows a comparison of the PES spectra of MgB_2 with those of gold measured under the same experimental condition. The leading edge of the MgB_2 spectrum at 15 K is shifted toward the high binding energy with respect to the gold reference, indicative of the gap opening at low temperature. On the other hand, the spectrum at 50 K looks to coincide with the gold reference within the present experimental accuracy, indicating that the gap is closed at 50 K with no pseudogap in contrast to the underdoped cuprate

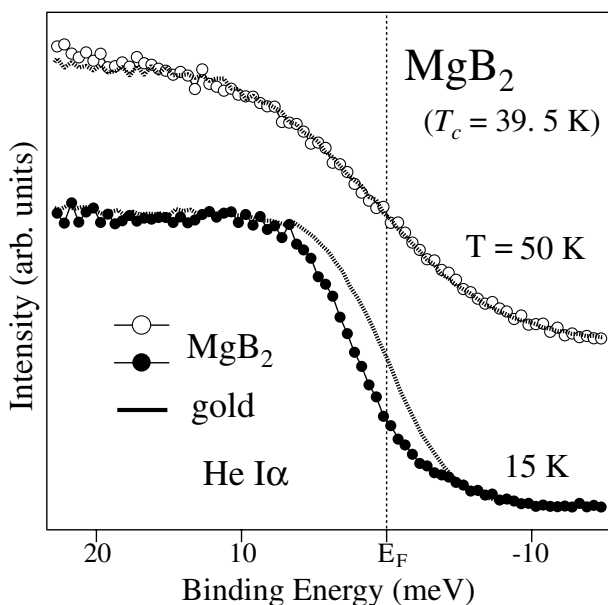


FIG. 2. Comparison of high-resolution PES spectra of MgB_2 with those of gold measured under the same experimental condition.

HTSCs [7,8]. We find that the leading edge of MgB_2 spectrum at 15 K is almost parallel to that of the gold reference, which suggests that the symmetry of the gap is s like and the gap size is within a few meV. In order to confirm this, we have performed numerical fittings to the PES spectrum and show the results in Fig. 3. In the simulation, we used the Dynes function [16] multiplied by the Fermi-Dirac function at $T = 15$ K and convoluted it with a Gaussian with a full width at half maximum (FWHM) of the instrumental resolution. We set the broadening parameter Γ to 1.1 meV. As shown in Fig. 3, the fittings with a d -wave gap of $\Delta = 5$ –10 meV seem to hardly reproduce the experimental PES spectrum at 15 K; both the coherent peak and the leading edge are not well reproduced simultaneously. On the other hand, the simulation with the s -wave gap of $\Delta = 4.5$ meV looks to fairly well reproduce the experimental curve. We found that the change of gap value by 0.5 meV in the fittings leads to an apparent deviation from the experimental spectrum. It is thus most probable that MgB_2 has an s -like superconducting gap and the gap value at 15 K is 4.5 ± 0.3 meV. The inset of Fig. 3 shows the gap value

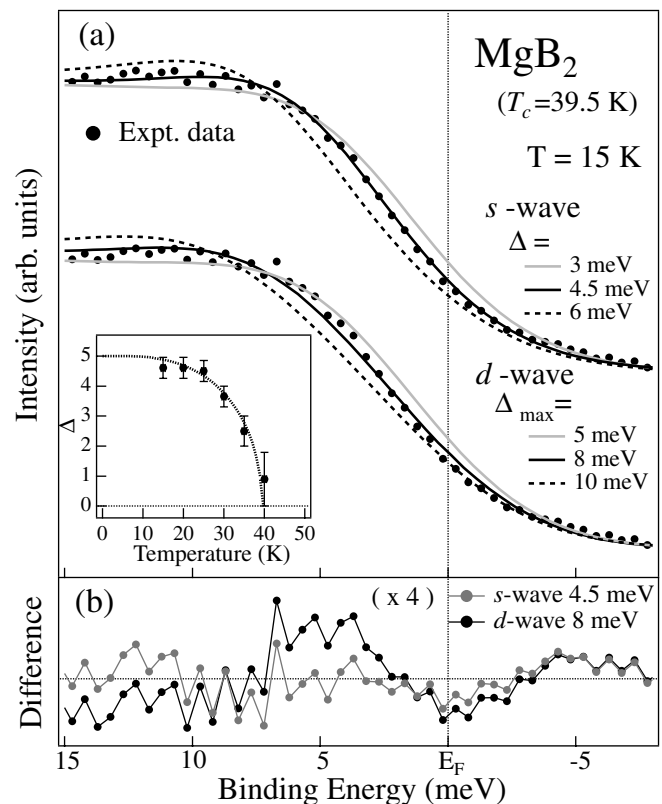


FIG. 3. (a) Results of numerical fittings to the high-resolution PES spectrum of MgB_2 at 15 K. The experimental spectrum is shown by filled dots and the fitting curves by lines. The inset shows the temperature dependence of the gap value obtained from the fittings to the PES spectra at several temperatures of 15–40 K. (b) Difference curves between the experimental spectrum and the representative numerical fitting curves based on s - or d -wave gap.

as a function of temperature obtained from the numerical fittings to the PES spectra measured at several temperatures of 15–40 K. The temperature dependence follows well the BCS form, suggesting the gap value at $T = 0$ to be about 5 meV. This gap value gives the ratio $2\Delta/k_B T_c$ of about 3, which is slightly smaller than the theoretical value (3.53) for a weak-coupling BCS superconductor [17]. All these strongly suggest that MgB₂ is categorized into a phonon-mediated BCS superconductor in the weak-coupling regime. It is inferred that high-frequency phonon(s) due to the light mass of boron atoms may cause the “high-temperature superconductivity” in MgB₂.

In conclusion, we have performed high-resolution photoemission spectroscopy on a newly discovered novel superconductor MgB₂. We have clearly observed opening/closure of a superconducting gap at E_F on decreasing/increasing temperature across T_c . The gap is found to be s like and the gap value (Δ) is estimated to be 4.5 ± 0.3 meV at 15 K from the numerical fittings to the PES spectra. The temperature dependence of the gap value is well described with the BCS form. The present PES results indicate that MgB₂ is categorized into a phonon-mediated BCS superconductor in the weak-coupling regime.

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