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Physica B 312–313 (2002) 150–151

PHYSICA B

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# Superconducting gap of $MgB_2$ observed using ultrahigh-resolution photoemission spectroscopy

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## Abstract

We study the superconducting gap of $MgB_2$ using high-resolution photoemission. In the spectrum measured at 5.4 K, a coherent peak with a shoulder structure is observed. We find that a simulation using two Dynes functions with the gap sizes of 1.7 and 5.6 meV reproduces the superconducting-state spectrum better than that using a single Dynes function and anisotropic Dynes functions. We also find that both of the smaller and larger gap close at the bulk transition temperature. These results indicate a multiple superconducting gap of $MgB_2$. © 2002 Elsevier Science B.V. All rights reserved.

*PACS:* 74.70.Ad; 74.25.Jb; 79.60.Bm

*Keywords:* Multiple superconducting-gap; PES; $MgB_2$

The recent discovery of the superconductivity at high-transition temperature ($T_c$), 39 K, in $MgB_2$ [1] has stimulated researcher's interest. One of the most important problems is whether the superconductivity of $MgB_2$ obey simple BCS theory or not. However, there is no sufficient explanation why $T_c$ is surprisingly high. Thus, we performed ultrahigh-resolution photoemission spectroscopy on polycrystalline $MgB_2$ in order to study the superconducting gap.

Fig. 1 shows photoemission spectra of $MgB_2$ measured at 5.4 K (open circles) and 45 K (open squares) with He I$\alpha$ resonance line. Details of sample preparation and measurement procedure are described elsewhere [2]. At 5.4 K we observe an intensity maximum at $\sim$7 meV and a shift of the leading edge, indicative of the opening of a superconducting gap. More importantly, we find a shoulder structure at 3.5 meV. These structures were not clearly observed in the recent photoemission study [3] most probably due to difference in experimental procedures and/or quality of the sample.

In order to get further insight into the shape of the superconducting gap, we analyzed the experimental spectra with the Dynes function [4] considering the Fermi–Dirac function at measured temperature and the known instrumental resolution. The Dynes function is a modified BCS function in the form of $D(E,\ \Delta,\ \Gamma) = Re\{(E - i\Gamma)/[(E - i\Gamma)^2 - \Delta^2]^{1/2}\}$ [4]. We actually found that both of the peak and shoulder structures were not fit at the same time using any sets of parameters in case of isotropic gap. Next, considering **k**-dependence of the gap, we try to fit all kind of anisotropic gap expected by group theory [5]. Again, we found that those structures were not fit with those functions. Supposing that the shoulder structure comes from another gap, we try to fit using the weighted sum of two Dynes functions ($D_{L+S}$) for a larger gap ($D_L$) and a smaller one ($D_S$), $D_{L+S} = (1/(1+R))D_L(E, \Delta_L, \Gamma) + (R/(1+R))D_S$

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PII: S0921-4526(01)01282-0

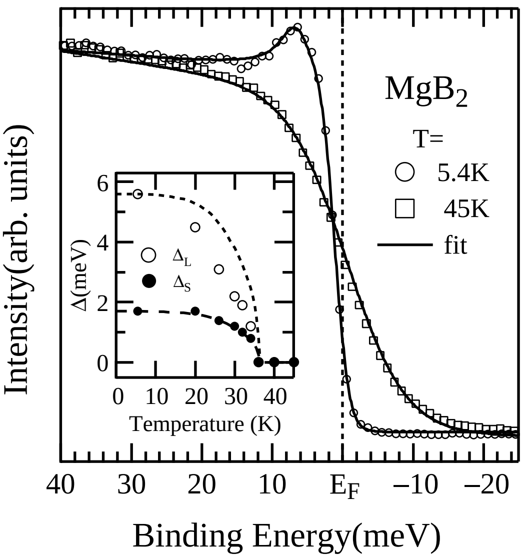


Fig. 1. Ultrahigh-resolution photoemission spectra of $MgB_2$ measured at 5.4 K (open circles) and 45 K (open squares) with He $I_\alpha$ resonance line (21.218 eV). Please note that the spectrum has a peak with a shoulder structure. The solid lines show the fitting results. Please see text about detail procedure to fit. The inset shows temperature dependence of the two gaps obtained from the analyses as described in the text. Filled and open circles represent the sizes of the smaller and larger gaps, respectively. Broken and dotted lines show the predicted temperature dependence of superconducting gap from BCS theory [6] for $\Delta(0) = 1.7$ and 5.6 meV, respectively.

$(E, \Delta_S, \Gamma)$, where $R$ is an amplitude ratio of the smaller gap to the larger one. The solid lines in Fig. 1 show the fitting results at 5.4 and 45 K. Here, we used the same value of $\Gamma$ for the two Dynes functions for simplicity. We succeeded in reproducing the experimental spectrum at 5.4 K using $\Delta_L = 5.6$ meV, $\Delta_S = 1.7$ meV, $\Gamma = 0.10$ meV and $R = 5.2$. These analyses show that the superconducting gap of $MgB_2$ is not a simple isotropic one, but rather contains two dominant components.

To see how the two gaps behave as a function of temperature, we analyzed temperature-dependent spectra assuming that $R$ is temperature independent. The inset of Fig. 1 shows obtained temperature-dependent gap values, where open and filled circles show the sizes of the larger and smaller gaps, respectively. Theoretical temperature dependence of gaps with $\Delta(0) = 1.7$ and 5.6 meV are also shown with broken and dotted lines, respectively [6]. We find, while the temperature dependence of the smaller gap follows the BCS prediction, that of the larger gap decreases faster than the prediction. We do not know the reason for the deviation so far, but the result is similar to that obtained from $MgB_2$/Ag and $MgB_2$/In junctions [7]. More importantly, both of the two gaps close at nearly the midpoint of $T_c$ (36.5 K) obtained from the magnetization measurements. From these results, we obtained the reduced gap size $2\Delta(5.4\,K)/k_B T_c$ of 3.56 for the larger gap and 1.08 for the smaller one.

Currently, there are active discussions on the mechanism of the superconductivity of $MgB_2$. Band calculations predict that Fermi surfaces in $MgB_2$ consist of quasi-two-dimensional band (hole like B-$2p_{xy}$ band or $\sigma$ band) and three-dimensional band (electron like B-$2p_z$ band or $\pi$ band) [8], and some theories indicate those may show different gap values [9]. Our result seems consistent to them. Further detailed studies to show calculated density of states are desired so as to be compared with the present study. From the present study, multiple gap is most likely, but to directly study the multicomponent gap and/or the anisotropy in relation to the bands, angle-resolved photoemission using single crystals are necessary and urgent.

In conclusion, we have measured high-resolution photoemission spectra on the superconductor $MgB_2$. We found the superconducting gap consist of two component and both of gaps close at the bulk transition temperature.

This work was supported by grants from the Ministry of Education, Culture and Science of Japan.

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