Abstract. We have performed systematic and comprehensive high-resolution angle-resolved photoemission (ARPES) measurements on Bi-system high-$T_c$ superconductors to study the quasi-particles related to and/or responsible for the occurrence of the superconductivity. We have experimentally determined the full energy dispersion and the coherence factors of the Bogoliubov quasi-particles, which show a good quantitative agreement with the prediction from the BCS theory. This proves the basic validity of the BCS theory in the broad sense to describe the high-$T_c$ superconductivity. We have experimentally identified two different bosonic modes in Bi-system high-$T_c$ superconductors. One produces a ‘small’ kink in the limited momentum region around the nodal cut and another is related to a ‘large’ kink which exists in a relatively wide momentum region with the stronger magnitude closer to the $(\pi, 0)$ point. The observed momentum and temperature dependence of the kinks as well as the impurity effect show that the large kink is of magnetic origin and closely related to the high-$T_c$ superconductivity.
1. Introduction

Recent remarkable improvement of the energy and momentum resolutions in photoemission spectroscopy has made it possible to directly observe the interaction between electrons and ‘modes’ in solids. Many physical properties of materials are well explained and formalized in terms of the properties of electrons dressed with the many-body interaction, named ‘quasi-particles’ (QPs). In this paper, we report results of high-resolution angle-resolved photoemission spectroscopy (ARPES) on Bi-system high-$T_c$ superconductors to study the many-body interaction responsible for and/or related to the occurrence of the superconductivity. Our first question in this study is whether or not the superconductivity in high-$T_c$ cuprates is understood in the framework of the BCS theory [1] in the broad sense. To answer this question, we have performed ultra-high resolution ARPES measurements on Bi$_2$Sr$_2$Ca$_2$Cu$_3$O$_{10+\delta}$ to directly observe the Bogoliubov quasi-particle (BQP) [2]. According to the BCS theory, the BQP is produced through the Cooper-pairing of two electrons and plays an essential role in characterizing the superconductivity. The experimental observation is regarded as the most direct evidence for the validity of the BCS-like mechanism of the superconductivity in high-$T_c$ superconductors. Once the BQP picture, in other words the BCS-like superconductivity in the broad sense is established, the next question is on the driving force of the superconductivity. In the BCS theory in the ‘narrow’ sense, it is a phonon (lattice vibration). From the beginning of the discovery of high-$T_c$ cuprates, the possibility of the phonon has been almost ignored or regarded as less important, simply because the superconducting transition temperature ($T_c$) exceeds far beyond the ‘BCS wall’ (40–50 K) predicted by the BCS theory in the narrow sense. However, recently, several theoretical and experimental studies have revived the role of the phonon and stirred a big debate with respect to the driving force of high-$T_c$ superconductivity. In order to get an insight into this essential problem, we have performed a systematic ARPES study on Bi-system high-$T_c$ superconductors, where we comprehensively measured the momentum- and temperature-dependence of the ‘kink’ in the energy dispersion near the Fermi level ($E_F$). Since the interaction of electrons with a certain bosonic mode (phonon, magnon, etc) responsible for the occurrence of superconductivity produces a QP near $E_F$ and appears as a ‘kink’ in the energy dispersion near $E_F$, each bosonic mode shows a characteristic momentum and temperature dependence of the kink, so that the systematic ARPES study would distinguish the origin of the kink (mode). Since it is expected that the kink feature shows a different response to an external disturbance such as impurity...
depending on different modes, we have studied the impurity effect on the kink to further clarify the origin.

2. Experiments

High-quality pristine Bi$_2$Sr$_2$Ca$_{n-1}$Cu$_n$O$_{2n+4}$ ($n = 2, 3$) single crystals and Ni-doped Bi$_2$Sr$_2$CaCu$_2$O$_8$ were grown by the travelling-solvent floating-zone (TSFZ) method. Details of sample preparations have been described elsewhere [3]. ARPES measurements were performed using a SCIENTA SES-200 spectrometer with a high-flux discharge lamp and a toroidal grating monochromator at Tohoku University, and with a same-type spectrometer at the undulator 4m-NIM beamline at the Synchrotron Radiation Center, Wisconsin. The He I$\alpha$ resonance line (21.218 eV) and 22 eV photons were used to excite the photoelectrons. The energy and angular (momentum) resolutions were set at 9–15 meV and 0.2° (0.007 Å$^{-1}$), respectively. Samples were cleaved in situ along the (0 0 1) plane in an ultrahigh vacuum better than $5 \times 10^{-11}$ Torr to obtain a clean surface. The Fermi level ($E_F$) of samples was referred to that of a gold film evaporated on the sample substrate.

3. Results and discussion

3.1. BQPs in Bi$_2$Sr$_2$Ca$_2$Cu$_3$O$_{10+\delta}$

Figures 1(a) and (b) shows ARPES spectra of overdoped Bi$_2$Sr$_2$Ca$_2$Cu$_3$O$_{10+\delta}$ (Bi2223, $T_c = 108$ K) at 140 and 60 K, respectively, measured along the cut in the Brillouin zone shown in the inset. Dark red coloured spectra are measured at $k_F$. (c) Same as (b) above $E_F$ in an expanded intensity scale. (d) Renormalized ARPES spectra at 60 K divided by the FD function at 60 K convoluted with a Gaussian representing the instrumental resolution.

Figure 1. (a), (b) ARPES spectra of overdoped Bi$_2$Sr$_2$Ca$_2$Cu$_3$O$_{10+\delta}$ (Bi2223, $T_c = 108$ K) at 140 and 60 K, respectively, measured along the cut in the Brillouin zone shown in the inset. Dark red coloured spectra are measured at $k_F$. (c) Same as (b) above $E_F$ in an expanded intensity scale. (d) Renormalized ARPES spectra at 60 K divided by the FD function at 60 K convoluted with a Gaussian representing the instrumental resolution.

New Journal of Physics 7 (2005) 105 (http://www.njp.org/)
in the inset. We clearly find that a superconducting gap of about 20 meV opens at the Fermi vector \((k_F)\) on lowering the temperature from 140 to 60 K across \(T_c\) and at the same time a sharp coherent peak grows up in the vicinity of \(E_F\) in the spectra. As the wave vector \((k)\) is changed from \((\pi, 0)\) to \((3\pi/2, -\pi/2)\), the coherent peak gradually disperses towards \(E_F\), showing a minimum energy gap at \(k_F\) (dark red coloured spectrum), which defines the superconducting gap and then disperses back to the higher binding energy by rapidly reducing its intensity. This spectral change below \(E_F\) is consistent with a previous ARPES result on Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi$_2$2212) \([4]\). More importantly, we find additional weak but discernible structures about 20 meV above \(E_F\) in the spectra, which are more clearly seen in figure 1(c) where the intensity scale is expanded. This new structure shows a clear momentum dependence with a stronger intensity in the region of \(|k| > |k_F|\), opposite to the behaviour of the band below \(E_F\). In order to see more clearly the band dispersion above \(E_F\), we have divided the ARPES spectra by the Fermi–Dirac (FD) function at 60 K convoluted with a Gaussian representing the instrumental resolution. The result is shown in figure 1(d), where we find a dispersive structure above \(E_F\) with a comparable intensity to that below \(E_F\), although the signal-to-noise ratio is relatively low because of the originally small ARPES intensity.

We plot in figure 2(a), the renormalized ARPES intensity (figure 1(d)) as a function of the momentum and the binding energy. Bright yellow and green areas correspond to the strong intensity in the renormalized ARPES spectra. We observe several characteristic behaviours for the two branches of dispersive bands: (i) the dispersive feature is almost symmetric with respect to \(E_F\) while the intensity is not; (ii) the energy separation of the two bands is minimum at \(k_F\); (iii) both bands show the bending-back effect at \(k_F\); and (iv) the spectral intensity of the two bands show the opposite evolution as a function of \(k\) in the vicinity of \(k_F\). All these features qualitatively agree with the behaviours of BQP predicted from the BCS theory \([1]\), indicating the basic validity of the BQP concept in high-\(T_c\) superconductors. Next, we compare the experimental result with the theoretical prediction to examine the quantitative validity of the BCS theory. We show in figure 2(a), the theoretical band dispersion of BQP (blue and red broken lines) for comparison. In the BCS theory, the band dispersion of BQP \((E_k)\) is expressed as

\[ E_k = (\epsilon_k^2 + |\Delta(k)|^2)^{1/2}, \]

where \(\epsilon_k\) and \(\Delta(k)\) are the normal-state dispersion and the superconducting gap, respectively. We have determined \(\epsilon_k\) (white solid line in figure 2(a)) from the ARPES spectra at 140 K. The superconducting gap \(\Delta(k)\) is assumed to be the \(d_{x^2−y^2}\)-wave superconducting order parameter \(\Delta(k) = \Delta_0|\cos(k_x) − \cos(k_y)|/2\), where \(\Delta_0\) is determined with a 60 K spectrum at \(k_F\). We find in figure 2(a) that the calculated dispersion traces well the strong intensity of ARPES spectra (yellow or green areas), showing a good agreement in the band dispersion between the experiment and the theory.

To further study the validity of the BQP concept, we compare the coherence factors above/below \(E_F\), \(|u_k|^2\) and \(|v_k|^2\), between the experiment and the theory. According to the BCS theory, the coherence factors are expressed as

\[ |u_k|^2 = 1 − |v_k|^2 = (1 − \epsilon_k/E_k)/2, \]

where \(\epsilon_k\) and \(E_k\) are the energy dispersion of the normal QP and BQP bands, respectively. We show these ‘theoretical’ coherence factors by smooth solid lines in figure 2(b). On the other hand, we experimentally deduced the coherence factors by fitting the original ARPES spectra with the

New Journal of Physics 7 (2005) 105 (http://www.njp.org/)
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Figure 2. (a) Plot of renormalized ARPES intensity (figure 1(d)) as a function of the momentum and the binding energy. Bright yellow and green areas correspond to the strong intensity in the renormalized ARPES spectra, showing the experimentally determined band dispersion of the BQPs. Blue and red broken lines are the theoretical band dispersions below and above \( E_F \), respectively, predicted from the BCS theory. Open circles show the experimental normal-state band dispersion, and the white solid line (\( \epsilon_k \)) is the fitting with a parabolic function.

(b) Comparison of the coherence factors above (\( |u_k|^2 \)) and below (\( |v_k|^2 \)) \( E_F \) between the ARPES experiment and the BCS theory.

The following equation:

\[
I(k, \omega) = I_0(k)\{A_{BCS}(k, \omega) + A_{inc}(k, \omega)\}f(\omega, T)@R(\omega),
\]

where \( I_0(k) \) is a prefactor which includes the kinematical factors and the dipole matrix-element. \( A_{BCS}(k, \omega) \) is the BCS spectral function expressed as,

\[
A_{BCS}(k, \omega) = \frac{1}{\pi} \left[ \frac{|u_k|^2\Gamma}{(\omega - E_k)^2 + \Gamma^2} + \frac{|v_k|^2\Gamma}{(\omega + E_k)^2 + \Gamma^2} \right],
\]
Figure 3. ARPES-intensity plot as a function of the wave vector and the binding energy for underdoped Bi$_2$Sr$_2$Ca$_2$Cu$_3$O$_{10}$ ($T_c = 100$ K), measured at the normal (140 K, upper panels) and the superconducting (40 K, lower panels) states for five cuts in the Brillouin zone (cuts 1–5) shown in the inset. Bright areas correspond to strong intensity in the spectra.

where $\Gamma$ is a linewidth broadening due to the finite lifetime of photoholes. $A_{inc}(k, \omega)$ in equation (3) is an empirical function to represent the incoherent background,$^2$ $f(\omega, T)$ is the FD function and $R(\omega)$ denotes the convolution with the resolution function $R(\omega)$. To remove the effect of $I_0(k)$, we have divided the spectral intensity of the superconducting state (60 K) with the integrated normal-state (140 K) spectral intensity at each $k$ point. We determined the peak weights below and above $E_F$ at each $k$ point by decomposing the spectrum, and then divided them by the average value of the total peak weight at each $k$ point.$^3$ We define these normalized weights as the experimental coherence factors $|\nu_k|^2$ and $|\mu_k|^2$ and have shown them in figure 2(b) with filled circles. As seen in figure 2(b), the coherence factors show a surprisingly good quantitative agreement between the experiment and the theory. It is also remarked that the sum of the experimental coherence factors is almost unity over the measured momentum region in good agreement with the prediction from the BCS theory, although the experimental coherent factors are determined totally independently of each other without using the sum rule. The present ARPES results indicate the basic validity of the BCS-like BQP picture in describing the superconducting state of high-$T_c$ cuprates.

3.2. Modes in Bi-system high-$T_c$ superconductors

Figure 3 shows ARPES-intensity plots as a function of the wave vector and the binding energy, namely the experimentally determined band dispersion, for underdoped Bi$_2$Sr$_2$Ca$_2$Cu$_3$O$_{10}$ ($T_c = 100$ K), measured at the normal (140 K) and the superconducting (40 K) states for five cuts in the Brillouin zone (cuts 1–5) shown in the inset. For cut 1 (nodal cut) at 40 K, a steep

$^2$ We assumed a linear background with a cutoff with respect to $E_F$ to represent the incoherent part of the spectra, as employed in previous ARPES studies on Bi2212 [5, 6].

$^3$ We did not use the normal-state quasiparticle weight for division, because the quasiparticle weight in ARPES spectrum shows temperature dependence in cuprates [5, 6].
band rapidly approaches $E_F$ from the high-binding energy side and slightly bends at 50–80 meV, showing a characteristic kink behaviour of the dispersion as reported previously [7]–[9]. As seen in figure 3, the small kink at 40 K in the nodal cut gradually grows up on approaching the $(\pi, 0)$ point and finally it becomes a gigantic kink in cut $\odot$ closest to $(\pi, 0)$. We also find that a superconducting gap of about 30 meV opens in the band dispersion in cut $\odot$. It is noted here that the observed gigantic kink in cut $\odot$ at 40 K is not due to the opening of the superconducting gap, because, as shown in the previous section, the BQP band bends smoothly rightward near $E_F$ in the layout of experimental data in figure 3 and does not make a kink like that in cut $\odot$. This indicates that the gigantic kink observed near $(\pi, 0)$ is intrinsic, showing the interaction of electrons with a certain bosonic mode. At this point, however, it is not clear whether the small kink at the nodal cut is continuously connected to the gigantic kink around the $(\pi, 0)$ point. This question would be resolved when we see the temperature dependence in figure 3. It is surprising that the gigantic kink in cut $\odot$ at 40 K totally disappears at 140 K above $T_c$ (100 K) as evidenced by the straight dispersive feature of the band, while the small kink in cut $\odot$ survives even above $T_c$ without changing the kink energy as seen in the upper panel of figure 3. It is also remarked that the small kink above $T_c$ is observed in a limited momentum region around the nodal cut, suggesting that the medium-sized kink observed in the momentum region between cuts $\odot$ and $\odot$ has the same origin as the gigantic kink in cut $\odot$. The observed clear difference in the temperature dependence indicates that the origin is different between the two kinks: one is a ‘small’ kink localized around the nodal cut and the other is a ‘large’ kink existing over a wide momentum region with the stronger amplitude closer to the $(\pi, 0)$ point. To investigate the origins of kinks, we have measured detailed temperature dependence of ARPES spectrum (band dispersion) for two representative cuts.

Figure 4 shows the temperature dependence of the experimental band dispersion along cuts $\odot$ and $\odot$. The gigantic kink at 30 K in cut $\odot$ is gradually weakened on increasing the temperature, almost disappears at $T_c$ (100 K) and then totally vanishes at slightly higher temperatures of 120–140 K, showing a good correlation with the temperature evolution of the superconductivity. In contrast, as seen in figure 4, the small kink in the nodal cut shows negligible temperature dependence although the kink looks slightly enhanced at low temperatures. The small kink does not show any noticeable change across $T_c$ (100 K) and survives at higher temperatures. The observed characteristic temperature and momentum dependence of the two kinks strongly suggests that the relatively strong kink in off-nodal cuts is closely related to the superconductivity, while the small kink localized around the nodal cut has no direct relation with the superconductivity. It is noted here that the magnetic resonance mode observed in the inelastic neutron scattering [10] has a momentum transfer of $(\pi, \pi)$, which connects two momentum regions of $(\pi, 0)$ and $(0, \pi)$, where the gigantic kink appears at low temperatures. The temperature evolution of the magnetic resonance mode is similar to that of the gigantic kink [10]. This suggests that the origin of the gigantic kink is magnetic and the same as that of the magnetic resonance mode. It is noted that the peak–dip–hump structure seen in Bi$_2$Sr$_2$CaCu$_2$O$_8$ [7] would be caused by the same mechanism as the kink around $(\pi, 0)$, since both the kink and the peak–dip–hump structure disappear above $T_c$. On the other hand, the origin of the small kink around the nodal cut may be different from that around the $(\pi, 0)$ point since the kink at the nodal cut survives above $T_c$. The optical phonon mode with the momentum transfer of $(\pi, 0)$ may explain the observed temperature dependence of the kink at the nodal cut [11].
3.3. Impurity effects on kinks and modes

In order to further clarify the origin of the kink in the dispersion, we have studied the impurity effect on the behaviour of the kink. It is expected that impurities such as Zn, Ni and Co affect substantially the magnetic environment in the CuO$_2$ plane while the lattice vibration is not so strongly influenced by the impurities with similar atomic weight. In fact, the magnitude of the $Q = (\pi, \pi)$ magnetic resonance mode observed by inelastic neutron scattering at the superconducting state is substantially weakened by impurity doping [12]. Figure 5 shows comparison of the Ni-impurity effect on the energy dispersion near $E_F$ between two different cuts in Bi$_2$Sr$_2$CaCu$_2$O$_8$. As seen in figure 5, the upturn of dispersion between 100 and 50 meV
is remarkably lost upon Ni doping. This shows the weakening of the kink structure around 50–80 meV. On the other hand, the kink in the nodal cut is hardly affected by the impurity. Almost similar results have been obtained in the cases of Zn or Co doping [13]. The present experimental result on the impurity effect shows that the large kink appearing near \((\pi, 0)\) has a close relation to the magnetic excitation, supporting the conclusion derived in the previous section. Since the impurity doping with Ni is known to totally suppress the superconductivity [14], it is inferred that the magnetic excitation which produces the large kink is essential for the occurrence of superconductivity.

4. Summary

We have performed high-resolution ARPES on Bi-system high-\(T_c\) cuprates to study the QP related to the occurrence of high-\(T_c\) superconductivity. We have succeeded in directly observing the full energy dispersion of the BQP formed via Cooper-pairing of two electrons at the superconducting state. We have also determined the coherence factors below and above \(E_F\) from the numerical fitting of the ARPES spectra. The experimentally determined band dispersion and coherence factors show a good quantitative agreement with the prediction from the BCS theory. This indicates the basic validity of the BCS theory in the broad sense to describe the superconducting state of high-\(T_c\) cuprates. The present systematic high-resolution ARPES study on the kink clearly identified two different bosonic modes in high-\(T_c\) cuprates, one of which produces a ‘large kink’ in the relatively wide momentum region with stronger amplitude closer to \((\pi, 0)\), and another is related to the ‘small’ kink located in a limited momentum region around the nodal cut. The large kink shows a close relation with the superconductivity in the temperature dependence, while no clear correlation is observed between the small kink and the superconductivity. Since the large kink has several common features such as momentum and temperature dependence with
the magnetic resonance mode, we conclude that both have the same magnetic origin responsible for the superconductivity. We observed that the large kink is substantially affected by the small amount (less than a few per cent) of magnetic impurity (Ni), while the small kink shows no impurity effect. This result confirms the magnetic origin of the large kink.

Acknowledgments

We thank T Fujii, T Watanabe, A Matsuda and K Kadowaki for supplying us high-quality single crystals. This work was supported by a grant from the MEXT of Japan.

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