a-b Plane Anisotropy of the Superconducting Gap in Bi$_2$Sr$_2$CaCu$_2$O$_8$: Scanning Tunneling Microscope Spectroscopy

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We have carried out electron tunneling spectroscopy on Bi$_2$Sr$_2$CaCu$_2$O$_8$ single crystals with use of STM at 4.2 K. The tunneling differential conductance in the superconducting gap was observed with varying tunneling direction in the a-b plane. Tunneling spectra observed along directions intermediate between Cu-O and Cu-Cu directions are well fitted with the $d_{x^2-y^2}$ wave model, taking into account the $\mathbf{k}$ dependence of the tunneling transition probability. This result strongly indicates that the superconducting gap has the $d_{x^2-y^2}$ wave symmetry with line nodes along the Cu-Cu direction.

Since the discovery of high-$T_c$ cuprates, many investigations have been carried out on the mechanism of its superconductivity. In high-$T_c$ cuprates, it is known that the superconductivity is caused by carriers in Cu-O layers, where the on-site Coulomb repulsive interaction at a Cu site is very strong. Therefore, the attractive interaction between electrons mediated by phonon can hardly bring about Cooper pairs in contrast to conventional superconductors. We must investigate the mechanism which causes an attractive interaction between electrons in such a strong correlation system. The symmetry of the superconducting pair wave function is an important clue to the attractive interaction between electrons. Many kinds of experiments were carried out to investigate it, e.g., measurement of the magnetic field penetration depth [1], angle-resolved photoemission spectroscopy (ARPES) [2,3], and NMR relaxation rate measurement [4]. Many of them suggest that the superconducting gap of high-$T_c$ cuprates has the $d$-wave symmetry. However, in the scanning tunneling microscope (STM) spectroscopy method, by which one can observe the electronic density of states directly with high resolution in energy, various results were reported [5–12], and those results have not converged yet. We reported that the superconducting gap is highly anisotropic in Bi$_2$Sr$_2$CaCu$_2$O$_8$ from STM spectroscopy measurements on single crystals [13]. In order to make more detailed discussion, we have observed tunneling differential conductance with varying tunneling direction in the a-b plane. In this article, we report the result of the tunneling spectra and discuss the symmetry of the pair wave function in the superconducting phase.

Bi$_2$Sr$_2$CaCu$_2$O$_8$ single crystals used in this study were grown by the floating-zone method. The superconducting transition temperature $T_c$ was determined as $T_c = 87$ K from the midpoint of the resistive transition. The crystal orientation was determined by x-ray diffraction. In this article, we always denote the [100] and [110] directions as the Cu-O bonding and Cu-Cu directions in the Cu-O plane, respectively. It was ensured that these single crystals grow along the [110] direction. Clean lateral surfaces were prepared by cutting them with a razor blade in air. Surfaces perpendicular to the [100], [110], and $\Phi = 9^\circ$, $19^\circ$, $27^\circ$, $35^\circ$, and $38^\circ$ directions from the [100] direction in the Cu-O plane were obtained. We ensured that each cut surface is flat with an optical microscope. Furthermore, we observed a typical cut surface with a scanning electron microscope (SEM) and ensured its flatness. The sample was mounted into the STM unit cell filled with the low pressure helium gas for thermal exchange. A mechanically sharpened Pt-Ir alloy wire was used as the STM tip. The measurements were carried out in the vacuum tunneling configuration where the STM tip does not contact to the sample surface. Differential conductance curves were observed directly by the lock-in technique with a 1-kHz ac modulation of 1 mV superposed on the bias voltage.

Typical differential conductance curves observed at 4.2 K with varying tunneling direction in the a-b plane are shown together in Fig. 1. The initial tunneling current $I_0$ is reduced exponentially with increasing the distance between the tip and the sample surface. We found that the functional form of the tunneling curves did not depend on the tip distance except for the [100] direction. Each curve is normalized by dividing with $I_0$ for the bias voltage $V_0 = 100$ mV. These curves show the clear superconducting gap structure except for the [100] direction. The curve along the [100] direction shows a conductance peak structure near zero bias voltage, whose detailed structure depends on the tip distance [14]. The functional form of curves along directions intermediate between [100] and [110] varies systematically, depending on the tunneling direction as described below. First, we discuss these curves from the viewpoint of the anisotropic superconducting gap.

For each tunneling direction, differential conductance curves were observed at several positions, which were aligned at intervals of about 10 nm on the cut surface. On each cut surface, essentially the same curve was observed...
The enhancement of the conductance near zero bias voltage is rather consistent with those obtained by other groups [8–12]. The functional form near zero bias voltage also shows the electronic density of states correctly inside the superconducting gap [13]. As shown in Fig. 1, the magnitude of the gap Δ depends only on the direction in k space, given as

\[ \Delta = \Delta_0 \cos 2\theta, \]

where Δ₀ and θ are the maximum value of the superconducting gap and the angle from the maximum gap direction in k space, respectively. The directional dependence of the tunneling differential conductance is given as

\[ \frac{dI}{dV}(V, \theta_0) \propto \int_0^{2\pi} \int_{-\infty}^{\infty} p(\theta - \theta_0) \times \text{Re} \left[ \frac{E - i\Gamma}{\sqrt{(E - i\Gamma)^2 - \Delta(\theta)^2}} \right] \times \left[ -\frac{\partial f(E + eV)}{\partial V} \right] N(\theta) dE d\theta, \]

where \( f(E) \) is the Fermi distribution function.

We try to fit these curves to the calculated electronic density of states with the \( d_{x^2-y^2} \)-wave model. We examine the simplest one, in which the gap Δ depends only on the direction in k space, given as

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\[
p(\theta - \theta_0) = \exp[-\beta \sin^2(\theta - \theta_0)]. \tag{3}
\]

The parameter \( \beta \) is given as

\[
\beta = \frac{2m}{\hbar^2} \frac{E_F}{\sqrt{U - E_F}} d, \tag{4}
\]

where \( U \) and \( E_F \) are the potential height of the tunneling barrier and the Fermi energy, respectively, and \( d \) is the width of the tunneling barrier. Owing to this factor, an electron whose kinetic energy component perpendicular to the tunneling barrier is large has a large probability of tunneling. The factor \( N(\theta) \) represents the anisotropy of the band dispersion and is given as

\[
N(\theta) = \frac{1}{|\nabla_k \varepsilon(k)|}. \tag{5}
\]

According to tight-binding approximation, the dispersion relation of the two-dimensional square lattice is given as

\[
\varepsilon(k) = \mu_0 - \varepsilon_0 \left[ \cos(k_x a) + \cos(k_y a) \right], \tag{6}
\]

where \( \mu_0, \varepsilon_0, \) and \( a \) are the Fermi energy in the half-filled conduction band, the bandwidth, and the lattice parameter, respectively. The direction dependence of \( N(\theta) \) is sensitive to the band filling. The conduction band of \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8 \), is almost half filled with a small amount of hole doping. We assume \( E_F - \mu_0 = -0.05\varepsilon_0 \) for the Fermi energy \( E_F \) in the following calculation. The value of \( N(\theta) \) calculated using this model has a large magnitude for the wave vector \( k \) around the [100] direction.

The differential conductance curves calculated for \( T = 4.2 \) K with this model are shown as broken curves in Fig. 3. In those fittings, we regarded \( \theta_0, \Delta_0, \) and \( \Gamma \) as fitting parameters for each direction. We fixed the parameter \( \beta \) as the value of 8 for all curves. The functional form near zero bias voltage of the calculated curve reproduces the flat behavior observed along near the [100] direction. The slope near zero bias voltage of the calculated curve becomes large with increasing \( \theta_0 \) and the energy-linear behavior observed along near the [110] direction is reproduced. Moreover, the functional form of the curve along \( \Phi = 38^\circ \), which is upwards convex inside the gap edge, is also well reproduced. The remaining conductance near zero bias voltage is explained by the broadening parameter \( \Gamma \). Small value of \( \Gamma = 0.3-1.1 \) meV assures the validity of the discussion about the superconducting electronic state with our tunneling curves. The variation of the enhancement of the gap edge, which is reduced with increasing \( \Phi \), is also well explained qualitatively. The gap width \( \Delta_{p-p} \) in the calculated curve using the same \( \Delta_0 \) becomes large with decreasing \( \theta_0 \). However, the values of the measured gap \( \Delta_{p-p} \) are not explained systematically with a unique value of \( \Delta_0 \). This implies that the sample dependence of \( \Delta_0 \) and the inhomogeneity of the sample are not negligible. The obtained values of \( \Delta_0 = 30-36 \) meV from the fitting are consistent with those of other tunneling experiments [8–12]. The value of \( \beta = 8 \), for which the transition probability decays by a factor of \( e^{-1} \) at \( \theta - \theta_0 = 20^\circ \), is relatively small. Ichimura et al. [16] reported the value of \( \beta = 20 \) from STM spectroscopy on (BEDT-TTF)\(_2\)Cu(NCS)\(_2\) which is an organic superconductor with the two-dimensional electronic band. As known from Eq. (4), this difference of the value of \( \beta \) is probably due to the difference of the work function \( U - E_F \) or the tip distance \( d \). In Fig. 4, the fitting parameter \( \theta_0 \) is plotted against \( \Phi \) measured under an optical microscope. These points are almost on the straight line which intersects the origin. This means that the line node of the gap is at the [110] direction. In the above fitting, an anisotropic band dispersion is assumed. We tried the same fitting assuming an isotropic band dispersion and ensured that these curves are well explained in the same way, and the similar relation between \( \theta_0 \) and \( \Phi \) is obtained again. Accordingly, our conclusion of the gap anisotropy does not depend on the assumed Fermi energy. Moreover, we ensured that all the curves which are shown in Fig. 2 are also explained by the \( d_{x^2-y^2} \)-wave gap in the same way. As a result, the
curves observed along the directions intermediate between [100] and [110] are well explained by the $d_{x^2-y^2}$-wave gap.

Shen et al. [2] observed the gap maximum along the [100] direction and observed the vanishing of the gap along the [110] direction in ARPES measurements on Bi$_2$Sr$_2$CaCu$_2$O$_8$ single crystals. The similar result was reported by Yokoya and Takahashi [3]. Although the existence of node is not ensured owing to the limit of the energy resolution, these results are consistent with ours. On the other hand, Kane and Ng [9] observed the gap minimum about 20 meV along near the [100] direction and observed the gap maximum about 35 meV along near the [110] direction, in STM spectroscopy on Bi$_2$Sr$_2$CaCu$_2$O$_8$ single crystals. At first sight, this result seems to indicate the $d_{s_y}$-wave symmetry and seems to be inconsistent with our result, which indicates the $d_{x^2-y^2}$-wave symmetry. We do not know the cause of this $\pi/4$ difference yet. However, the gap value is sample dependent, as described above. We think that our conclusion based on the functional form of conductance curves is highly conclusive.

As shown in Fig. 1, the so-called zero-bias conductance peak (ZBCP) structure [17] was observed along the [100] direction, and a clear superconducting gap structure was observed along the [110] direction. The ZBCP structure was reported also by other groups for the tunneling spectroscopy curves observed along the directions intermediate between [100] and [110] are well fitted with the $d_{x^2-y^2}$-wave gap model, taking into account the $\mathbf{k}$ dependence of the tunneling transition probability. This strongly indicates that the pair wave function has the $d_{x^2-y^2}$-wave symmetry.

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