Observation of an inelastic scattering mode by scanning tunneling spectroscopy on NdBa$_2$Cu$_3$O$_x$

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Abstract. We report the results of inelastic electron tunneling spectroscopy (IETS) on the $ab$ plane ($c$-axis tunneling) of a slightly underdoped twinned NdBa$_2$Cu$_3$O$_x$ single crystal ($T_c = 93.5$ K) performed with a scanning tunneling microscope at $T = 4.2$ K. In the energy derivative ($d^2I/dV^2$) of the differential conductivity curves having coherence peak, dip and hump structures, we observe a resonance peak at 24±2 meV. Here we discuss the possible origin of this inelastic scattering peak.

1. Introduction

In high-$T_c$ superconductors (HTSC) the interaction that mediates the pair formation is still one of the main unresolved issues. In several inelastic neutron scattering (INS) and angle resolved photoemission (ARPES) experiments a resonance peak was observed which suggested an important role played by collective spin excitation modes in HTSC [1-3]. However, there are also recent ARPES experiments which indicate an electronic coupling with the phonons producing kinks in the dispersion curves [4,5]. From these INS and ARPES experiments on YBa$_2$Cu$_3$O$_7$ (YBCO) and Bi$_2$Sr$_2$CaCu$_2$O$_8$ (Bi-2212) a consensus has been reached that coupling of electrons to a certain bosonic mode plays an important role in HTSC. But whether this boson is a phonon or a collective spin excitation mode is still not resolved.

In conventional superconductors, tunneling spectroscopy experiments were very useful in establishing the role of phonons in pair formation [6]. Jaklevich et al. showed that during tunneling if the energy of the electrons exceeds the local vibrational mode energy a new scattering channel evolves due to inelastic scattering of electrons resulting in a kink in the tunneling conductivity data [7]. A low temperature scanning tunneling microscope (STM) was successfully used by Stipe et al. to perform inelastic scanning tunneling spectroscopy (IETS) to elucidate the local single molecule vibrational modes on metal surfaces [8]. Based on the success of this experiment, Balatsky et al. recently suggested that STM can be used to observe bosonic modes that might be coupled to the electrons in HTSC [9].

In this work we report on IETS studies on a slightly underdoped NdBa$_2$Cu$_3$O$_x$ (NdBCO) single crystal. NdBCO is an important member of the 123 HTSC family, which has an identical unit cell structure as YBCO apart from the presence of Nd$^{3+}$ ions instead of Y$^{3+}$. Nd$^{3+}$ has a magnetic moment unlike Y$^{3+}$. However, there is no evidence of any interaction between Nd$^{3+}$ ions and Cu$^{2+}$ ions in the NdBCO unit cell [10]. Thus in NdBCO the CuO$_2$ plane (Cu-O plane layer) which is responsible for superconductivity is electronically in similar environment to that in YBCO. It was reported that the
NdBCO surface is chemically very stable which is important for STM experiments [11]. In our experimental data, a clear resonance peak is observed at 24±2 meV in all the energy derivatives of the differential conductivity curves having coherence peak and beyond the peak, dip and hump (PDH) structures which are well known to be the typical feature of the superconducting density of states in HTSC [12-14]. The resonance peak observed in our experiments on NdBCO suggests that there is a coupling of electrons to a certain bosonic mode which thus supports that this coupling plays an important role in HTSC.

2. Experiments

Very pure, stoichiometric NdBa$_2$Cu$_3$O$_{7-δ}$ single crystals were grown from a BaO/CuO flux in SnO$_2$ crucibles by the slow-cooling method [15]. Powders of Nd$_2$O$_3$, BaCO$_3$ and CuO of purity better than 99.99% were used. The growth was performed in air at a pressure of 70 mbar. Crystal growth started at 1283 K, and the cooling rate during growth was 0.40 K/h. At the end of the growth process the remaining flux was poured off within the furnace and then cooled down to room temperature under reduced pressure. Finally, the crystals have been oxidized at 593 K for 185 h in an atmosphere of 580 bar of O$_2$. The superconducting transition of the crystal was found by ac susceptibility at $T_c = 93.5$ K showing that the sample is slightly underdoped. The crystal was also characterized by X-ray diffraction and has been found to have a single phase.

The scanning tunneling spectroscopy (STS) experiments have been performed on the $ab$-plane using a home-made low temperature STM [16]. The as-grown annealed sample is cleaned with absolute ethanol and then dried with highly pure He gas. It is then immediately loaded into the STM and kept under He exchange gas at atmospheric pressure. The sample is then slowly cooled to 4.2 K. The experiments are performed under He gas atmosphere. The STM tip is a mechanically cut Pt-Ir (90-10) wire.

The differential conductance ($dI/dV$) curves are obtained against the bias voltage for which the bias is ramped while keeping the tip-sample distance constant. For the $dI/dV$ curves, we employed a lock-in amplifier with modulation voltage of 1 mV at a frequency of 1 kHz added to the bias voltage. $dI/dV$ curves are obtained at every 0.5 nm of a 32 × 32 nm$^2$ area with a very slow bias ramp. Each curve is taken in ~ 1 min. The STS experiments are performed at a tunnel set point of 100 mV and 0.1 nA. The spatial reproducibility of the curves show that the tunnel junctions formed by the Pt-Ir tip and the sample during the entire experiment are very stable.

3. Results and discussion

In the entire scan range we have observed $dI/dV$ curves which represent both superconducting and nonsuperconducting regions. The $dI/dV$ curves representing the superconducting state have the typical PDH structures. A representative curve is shown in Fig. 1(a). The nonsuperconducting curves are identified as the ones having no clear PDH structures. In this work we are concerned only with the $dI/dV$ curves which represent a superconducting state.

In the $dI/dV$ curves, we observe that there is an asymmetry in the peak positions and also the peak height. The peak-height asymmetry is related to the particle-hole asymmetry in the hole-doped cuprates [17]. We believe that the asymmetry in the peak position also arises due to the same reason.

In Fig. 1(b), the derivative ($d^2I/dV^2$) of the curve in Fig. 1(a) is plotted against the bias voltage. In the $d^2I/dV^2$ curve, we observe a resonance peak at an energy beyond the coherence peak position, both at the empty and filled states. This peak corresponds to a small kink in the slope beyond the coherence peaks in the $dI/dV$ curves as shown by the arrows in Fig. 1(a). Interestingly, these kinks are present in the curves where there are clear PDH structures observed.

In case of conventional superconductors, using strong coupling theory Eliashberg predicted that electron-phonon interactions would affect the superconducting DOS at an energy $E = \Delta + \Omega$, where $\Delta$ is the superconducting energy gap and $\Omega$ is the energy of phonons [18]. Rowel et al. in their tunneling experiments on conventional superconductors indeed proved the phonon contribution at the phonon energy $\Omega$ [6]. Recently Balatsky et al. showed that an inelastic scattering of electrons off a local
phonon or a spin in \textit{d}-wave superconductors would result in a kink-like singularity in the density of states \cite{9}. In the STS experiment, this kink in the \(dI/dV\) curve leads to a step in the \(d^2I/dV^2\) at an energy of \(E = \Delta + \Omega\). From our experimental data, considering \(\Delta\) as the coherence peak position, we find that \(2\Delta = 70.6 \pm 1.5\) meV. It is interesting to note that although there is an asymmetry in the coherence-peak position with respect to the bias (i.e., asymmetry with respect to empty and filled sample states) \(E-\Delta\), that is, \(\Omega\) is symmetric with respect to the bias. \(\Omega\) ranges from 20 meV to 28 meV with its mean value being 24 meV with a standard deviation of 2 meV. This is shown as a histogram plot in Fig.2.

**Figure 1:** (a) A representative \(dI/dV\) curve showing coherence peak, dip and hump structures beyond the peak obtained in the \(c\)-axis tunneling on a NdBa\(_2\)Cu\(_3\)O\(_x\) single crystal. The coherence peaks are broadened and the gap is not complete which is typical of HTSC. (b) Derivative of the curve shown in (a) where the resonance peaks in empty and filled states corresponding to the kinks in \(dI/dV\) are shown by arrows.

We note that our finding on NdBCO is the first report of a resonance peak at \(\sim 24\) meV energy observed in STS experiments in the 123-HTSC family. The origin of this resonance is not clear. In neutron scattering experiments on optimally doped YBCO, a sharp resonance in the superconducting state was observed at an energy of 41 meV \cite{2,19}. In an underdoped YBCO, Dai \textit{et al.} observed a peak at 34 meV \cite{20}. Their experiments suggested that the peaks are due to inelastic scattering of electrons off a collective spin-excitation mode at those energies. On the other hand, from the ARPES experiments along the nodal direction on Bi-2212, La\(_{2-x}\)Sr\(_x\)CuO\(_4\) and Pb-doped Bi-2212, Lanzara \textit{et al.} showed that an electron-phonon interaction is responsible for a kink in the dispersion curve in an energy range of 50-80 meV \cite{4}. From our IETS data, the origin of the resonance peak at \(\sim 24\) meV can not be estimated. However, we note that we observe this peak in \(d^2I/dV^2\) curves corresponding to all the \(dI/dV\) curves containing PDH features. These PDH features have been systematically observed in tunneling and ARPES experiments on Bi-2212 and have been established as important characteristics of a \(dI/dV\) curve on high-\(T_c\) cuprates \cite{12-14}. In STS experiments, these typical features are observed when the electron tunneling takes place from the Cu-O plane layer. In our experimental data on NdBCO, we observe all these typical features thus confirming that the tunneling takes place between the normal conducting tip and the Cu-O plane layer that is responsible for superconductivity. This suggests that the resonance peak we observe at \(\sim 24\) meV must be due to an inelastic interaction of electrons arising out of coupling to some mode originating in the Cu-O plane layer. The possible phonon modes in this plane at around this energy are the out of plane vibration of oxygen atoms (B\(_{\text{lg}}\)
phonons) or in plane stretching mode vibration of oxygen atoms and a collective spin excitation mode. Cuk et al. has reported the observation of the B_{1g} mode coupling in Y-doped Bi-2212 at 40 meV [5]. A detailed doping and temperature dependent study will be useful to elucidate more information on these modes. From an a-axis tunneling experiment on an optimally doped ($T_c = 95.5$ K) NdBCO single crystal, we observed a similar resonance peak in the $d^2I/dV^2$ curve at an energy of ~ 35 meV (not shown here). To establish whether a clear doping dependence of $\Omega$ exists or not, studies on underdoped samples will be important.

![Figure 2](image.png)

**Figure 2.** Histogram showing the spread of $\Omega$ values obtained from the derivative of the entire set of $dI/dV$ data with peak, dip and hump structures. It is calculated as $E-\Delta$ in accordance with the strong coupling theory. $\Omega$ has a mean value of 24 mV and a standard deviation of 2 mV.

4. Conclusion
On a slightly underdoped NdBCO single crystal, from tunneling experiments a resonance peak was observed in the $d^2I/dV^2$ curve. The peak is the result of inelastic scattering of electrons off some scattering mode. Our data shows that a 24 meV peak is an important feature of this NdBCO and suggests that the kinks in the dispersion curves in ARPES and peaks in neutron scattering experiments on Bi-2212 and YBCO might be of similar origin. Although our results do not provide a clue regarding the origin of the coupling mode, however, we show that IETS with STM can be used to study the strong coupling of electrons in HTSC. It also shows that these resonance peaks due to inelastic scattering of electrons are present in general in all HTSC thus underlining its role in superconductivity.

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