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Line-shape analysis of the Raman-spectrum from B_{1g} bond buckling phonon in $Bi_2Sr_2CaCu_2O_{8+x}$

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Abstract

We performed Raman spectroscopy on two different over-doped $Bi_2Sr_2CaCu_2O_{8+x}$ (BSCCO), of which superconducting transition temperatures are 89 K and 77 K. Line-shape analysis of the Raman-spectrum was done, focused on B_{1g} bond buckling mode which have drawn a lot of attention, since photoemission studies showed an evidence for strong coupling between the mode and electron. The line-shapes show asymmetry and are well fitted by the Fano line-shape formula. Remarkably, we found that the peak line-widths from B_{1g} bond buckling mode in BSCCO show much broader than those in $YBa_2Cu_3O_{7-x}$. The broad line width can be attributed to the superstructure modulation of BSCCO. Our results imply that B_{1g} bond buckling mode may have close relation to the origin of superconductivity or to boosting the superconducting transition temperature in BSCCO.

Keywords: high temperature superconductivity, cuprate, $Bi_2Sr_2CaCu_2O_{8+x}$, B_{1g} bond-buckling phonon, Raman spectroscopy

1. INTRODUCTION

It has been pursued for a long time to reveal the origin of high temperature superconductivity (HTS) since the discovery of HTS in $La_{2-x}Ba_xCuO_4$ [1]. People realized from the unusual isotope effects in HTS that the HTS is not a conventional superconductivity in which phonon mediates the Cooper pairs [2]. Spin fluctuations, charge density fluctuations as the possible candidates replacing phonons in the BCS theory for mediating the Cooper pairs have been also intensively studied [3, 4].

In 2004, the B_{1g} bond-buckling phonon in $Bi_2Sr_2CaCu_2O_{8+x}$ (BSCCO) drew a lot of attention, since angle resolved photoemission spectroscopy (ARPES) show strong electronic band dispersion anomaly at about 40 meV binding energy in BSCCO [5], and this was interpreted as an evidence for coupling between the B_{1g} bond-buckling phonon and electron [6]. The B_{1g} bond-buckling phonon has been also recently proposed to play a crucial role in origin of HTS along with the electron-electron correlation from the ARPES studies of over-doped BSCCO [7]. They found that electronic band dispersion anomaly at about 40 meV binding energy is rapidly reduced as superconducting transition temperature rapidly decreases in over-doped region [7]. It is desired to measure doping dependent phonon spectrum in over-doped BSCCO, in order to investigate coupling strength between the B_{1g} bond-buckling phonon and electron from phonon as well.

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Raman spectroscopy is a powerful tool to measure the B_{1g} bond-buckling phonon of cuprate HTSs [8]. While the B_{1g} bond-buckling phonon in $YBa_2Cu_3O_{7-x}$ (YBCO) has been intensively studied by Raman spectroscopy [9, 10], that of BSCCO has not been much studied, especially for doping dependence in over-doped region. In this article, we report doping dependent Raman spectroscopy in over-doped BSCCO. The line-width of Raman peak from the B_{1g} bond-buckling phonon shows very broad. The broad line width can be attributed to the superstructure modulation of BSCCO. The implication for origin of HTS in BSCCO is discussed.

2. EXPERIMENTAL DETAILS

High quality BSCCO single crystals were synthesized by the floating zone method. Hole doping concentration of BSCCO can be controlled by post-annealing process. We prepared two different hole doped BSCCO through different conditions of post-annealing process. One is slightly over-doped BSCCO (OD89) of which transition temperature (T_c) is 89 K. The other is moderately over-doped BSCCO (OD77) of which T_c is 77 K. Here, T_c is defined as the temperature showing the half of saturated diamagnetic susceptibility (inset of Fig. 1 bottom).

High resolution and low energy cut-off Raman has been performed on two different doping concentrated BSCCO and YBCO as well for comparison. Temperature of the samples inside optical cryostat was varied from room temperature down to about 68 K by liquid nitrogen cooling.

3. RESUTS AND DISCUSSION

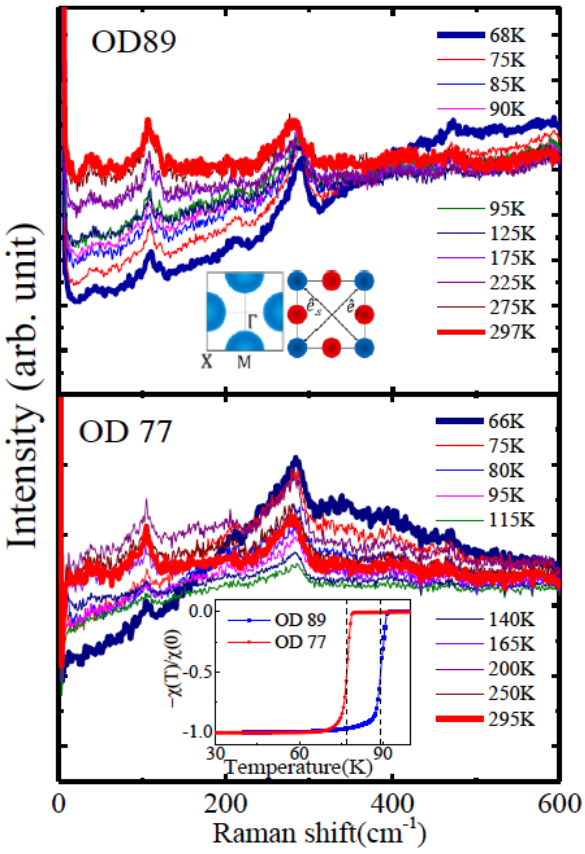

Fig. 1. Temperature dependent Raman spectrum for slightly over-doped BSCCO (OD89) and moderately over-doped BSCCO (OD77). The inset of the top figure indicates the polarization of incident light ($\mathbf{e}_i$) and scattered light ($\mathbf{e}_s$). Blue and red balls indicate copper and oxygen atoms on copper oxide plane of BSCCO, respectively. This combination of light polarizations is for B_{1g} symmetry excitations in BSCCO. The inset of the bottom figure is magnetic susceptibility as a function of temperature showing the Meissner effect and superconducting transition temperatures (vertical dashed lines) of OD89 and OD77.

Fig. 1 shows the temperature dependent Raman spectrum. Polarizations of incident and scattering lights are perpendicular to each other and the polarization of incident light is 45 degree about the copper-oxygen bonding direction (inset of Fig. 1 top). This combination of light polarizations is for the B_{1g} symmetry excitations in BSCCO. Raman spectrum from both OD89 and OD77 show at least two sharp peaks at about 100 cm^{-1} and at about 280 cm^{-1}. The peak at about 280 cm^{-1} shows stronger intensity and broader than the other at about 100 cm^{-1} and is from the B_{1g} bond-buckling phonon [11]. The clearest character of temperature evolution of Raman spectrum is from broad background signal originating from electronic Raman process. Backgrounds of the highest temperature data is rather flat, but backgrounds of the lowest temperature data (68 K for OD89 and 66 K for OD77) show very different, and are less at small Raman shift and more at large Raman shift. This kind of characteristic evolution is due to the formation of the d-wave superconducting gap at below T_c in BSCCO [11]. The electronic Raman intensities are enhanced at the energy of about superconducting gap size, 2Δ, and are suppressed below the energy. Therefore, 2Δ of OD89 and OD77 should be about 500 cm^{-1} and 300 cm^{-1}, respectively.

Raman spectrum for the B_{1g} bond-buckling phonon will be focused as shown in Fig. 2, since motivation of Raman study is to investigate the coupling strength between the B_{1g} bond-buckling phonon and electron. The peaks clearly show asymmetry and fit well to the Fano-line formula, which reads,

$$I_F = \frac{I_0\left[\left(q+\frac{\omega-\Omega}{\Gamma}\right)^2\right]}{\left[1+\left(\frac{\omega-\Omega}{\Gamma}\right)^2\right]}$$

There are three parameters, Ω, Γand q, which are directly related to peak position, line width and asymmetry, respectively. The larger absolute value of the inverse number of q shows the more symmetric line-shape. The Fano-line functions fitting to the data are shown together with the Raman spectrum in Fig. 2 (c) and (d). The parameter values, which produce the Fano-line functions, are also shown in the figure. The asymmetric line-shape can originate from the coupling to the continuum states such as electronic continuum [12]. Line width, Γ, is proportional to the scattering rate of the mode. Line width should be bigger with stronger coupling to electron.

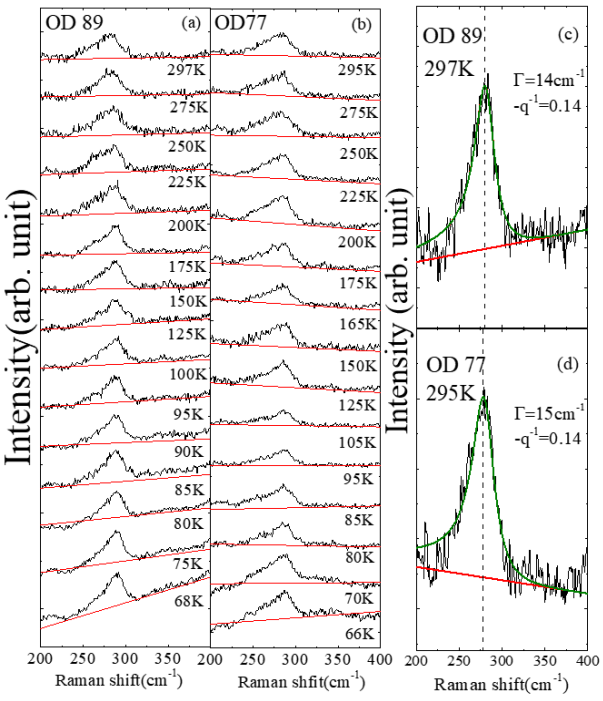

Fig. 2. Temperature dependent Raman spectrum in smaller range of Raman shift focusing on the peak of the B_{1g} bond-buckling phonon for OD89 (a) and for OD77 (b). Red lines indicate the background. (c) and (d) are Raman spectrum with the Fano line formula fitting to the spectrum. Vertical dashed lines indicate the peak positions.

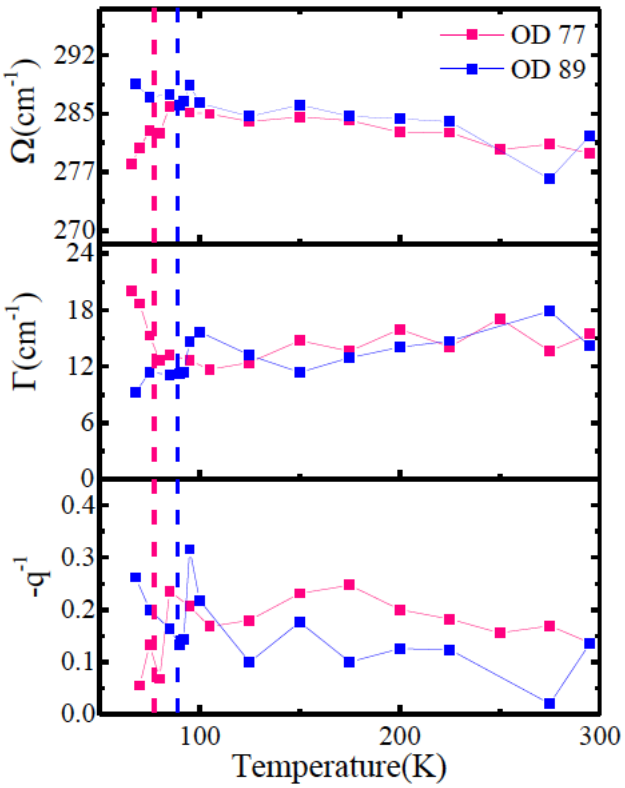

Fig. 3. Three fitting parameter values of the Fano-line function, Ω, Γ and $-q^{-1}$ as a function of temperature. The vertical dashed lines indicate the T_cs for OD89 and OD77.

Three fitting values for the Raman peaks for the B_{1g} bond-buckling phonon are shown in Fig. 3. Peak positions and line widths of OD89 and OD77 are similar to each other above about 100 K. However, temperature dependences between two become very different bellow about 100 K. Line-widths of OD77 become bigger, while those of OD89 rather become smaller as decreasing temperature below about 100 K. Peak positions of OD77 become lower, while those of OD89 rather become higher as decreasing temperature below about 100 K. This different behavior is probably due to the different superconducting gap size (2Δ) between two. The energy of the B_{1g} bond-buckling phonon is well below 2Δ for OD89 and is similar to 2Δ for OD77.

Line-shape analysis indicates that there may be finite coupling between the B_{1g} bond-buckling phonon and electron, since the line-shape show asymmetry and broad line-width. Please note in Fig. 1 that the peak from the B_{1g} bond-buckling phonon at about 280 cm^{-1} is much broader than the other peak at about 100 cm^{-1}. However, the line-widths are remarkably similar regardless of doping concentrations above 100 K, although the line-widths are expected to be much smaller in OD77 than in OD89, since ARPES study reported that the coupling between the phonon and electron becomes much smaller in OD77[6]. One may consider the other origin dominantly contributing to the broad line-width in BSCCO regardless of doping concentration.

Superstructure modulation in BSCCO, which may originate from the lattice mismatch between copper oxide layer and bismuth oxide layer in BSCCO, has been known for a long time [13, 14]. Scanning tunneling spectroscopy (STS) study revealed that superconducting gap size is also spatially modulated along with the superstructure modulation in BSCCO [15]. One can imagine that the superstructure modulation causes many different mode energies of the B_{1g} bond-buckling phonon and in turn produce broad line-shape. We can notice that the line-shape from the B_{1g} bond-buckling phonon in YBCO, which has no superstructure modulation, shows much sharper (Fig. 4).

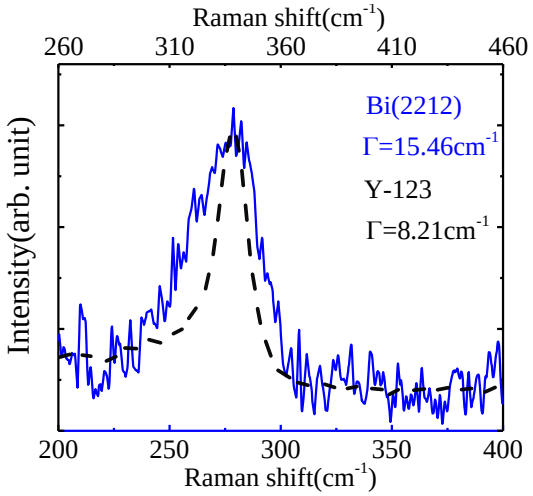

Fig. 4. Raman spectrum of BSCCO (OD77) and YBCO at room temperature showing the peak by the B_{1g} bond-buckling phonon. The bottom and top horizontal axes are for BSCCO and YBCO, respectively.

Our results provide a possible experimental evidence that the B_{1g} bond-buckling phonon has local nature by superstructure modulation in BSCCO and its mode energy is sensitive to local position inside the unit cell of the superstructure. STS results also show that superconducting gap locally varies inside the unit cell of the superstructure. Therefore, our results imply that the B_{1g} bond-buckling phonon is a possible candidate responsible to the local variation of superconducting gap and the B_{1g} bond-buckling phonon may play important role in BSCCO.

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