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A systematic optical study of phonon properties in optimally doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystals

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Abstract

A systematic optical study of infrared-active phonons is carried out for optimally doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) single crystals with *E*-vector along *c*-axis as well as in the *ab*-plane at 295 K. Strong phonon anisotropy has been observed in our *ab*-plane conductivity measurements. Ten infrared-active phonons have been observed along *c*-axis. Many of these *c*-axis infrared-active phonons have energies that are very close to the Raman-active A_{1g} modes. The group theory analysis based on the tetragonal group (D_{4h}) is inadequate to explain our experimental observations.

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1. Introduction

In view of the renewed suggestion that strong electron-phonon interaction [1] is the mechanism for superconductivity in high T_c cuprates, phonon properties need to be examined more carefully in these systems. Phonons in high T_c cuprates has been the focus of many Raman works [2]. The vibrational spectra of high T_c cuprates are difficult to interpret and this is particularly true in the case of $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) with the presence of a structural modulation [3]. Infrared spectroscopy might shed some light on these questions. Using the vibrational spectra derived from both the infrared and Raman spectroscopy, a more complete understanding of phonon properties of Bi2212 can be reached. Group theory analysis based on a tetragonal cell (space group D_{4h}) in Bi2212 [4], gives 30 modes at the center of the Brillouin zone for Bi2212 [5]: $\Gamma \equiv 6A_{1g} + B_{1g} + 7E_g + 7A_{2u} + 8E_u + B_{2u}$. Of the total of 30 modes: two are acoustic ($A_{2u} + E_u$) and therefore not infrared or Raman-active; thirteen ($6A_{2u} + 7E_u$) are infrared-active; fourteen ($6A_{1g} + B_{1g} + 7E_g$) are Raman-active and one is silent (B_{2u}).

The *ab*-plane optical conductivity of optimally doped Bi2212 single crystals has been measured extensively [6,7], but no lattice modes have been observed directly. However, only one brief study on the *c*-axis conductivity in Bi2212 was reported [8]. In this paper, a systematic optical study of infrared-active phonons is carried out for optimally doped Bi2212 single crystals with *E*-vector

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along c-axis as well as in the ab-plane at 295 K. Strong phonon anisotropy has been observed in our ab-plane conductivity measurements. Ten infrared-active phonons have been identified along c-axis. Many of these c-axis infrared-active phonons have energies that are very close to the Raman-active A_{1g} modes. The group theory analysis based on the tetragonal group (D_{4h}) is inadequate to explain our experimental observations.

2. Experimental details

For this study, large optimally doped Bi2212 single crystals are grown using traveling-surface-floating-zone (TSFZ) method [9]. The Bi2212 single crystals are mounted on an optically black cone, and the reflectance is measured in a near-normal-incidence arrangement from $\sim 50\,cm^{-1}$ to over $20{,}000\,cm^{-1}$ on a Bruker IFS 66v/S. The resolution of this infrared work is $2\,cm^{-1}$ in the phonon region. The absolute reflectance is determined by evaporating a gold film (~ 100 nm in thickness) in situ in an ultra-high vacuum ($\sim 1 \times 10^{-8}$ Torr). This comparison to the gold reflectivity provides an absolute reflectivity scale. The details of this technique are described elsewhere [10].

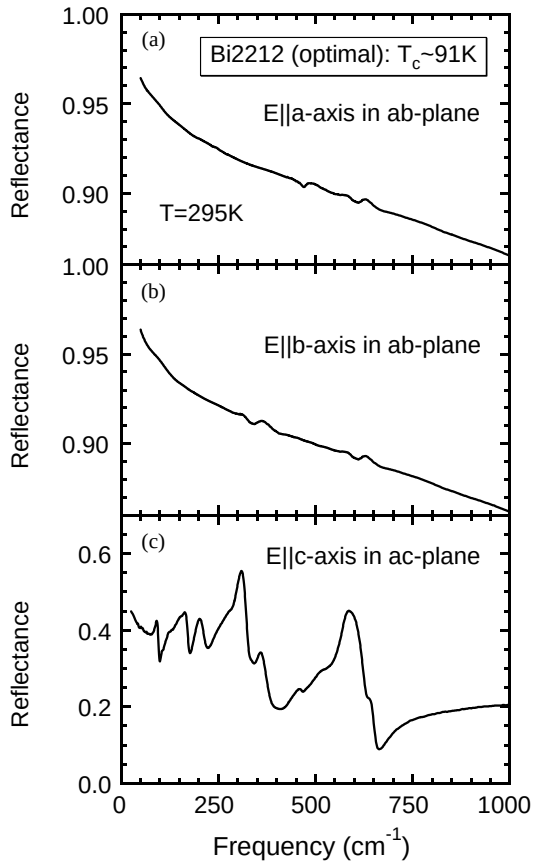

Fig. 1. The measured low frequency reflectance of optimally doped Bi2212 single crystals with the E-vector parallel to a, b and c-axes at 295 K. (a) The reflectance with $E \| a$-axis in ab-plane; (b) the reflectance with $E \| b$-axis in ab-plane; and (c) the reflectance with $E \| c$-axis in ac-plane.

3. Experimental results and discussion

In Fig. 1, reflectance spectra are shown for optimally doped Bi2212 single crystals with E-vector parallel to a, b and c-axes at 295 K. In Fig. 1(a) and (b), the low frequency ab-plane reflectance spectra are given. Because of the unprecedented high signal-to-noise ratio (~ 1000) achieved using our in situ evaporation technique, structures due to infrared-active ab-plane phonons have been observed for the first time in optical measurements of optimally doped Bi2212. The reflectance for $E \| b$-axis is about 0.3% lower than that of for $E \| a$-axis in this frequency region consistent with the previous observations [7]. The reflectance spectrum for $E \| c$-axis is shown in Fig. 1(c). Many phonon features can be observed in the c-axis reflectance spectrum.

We have measured the reflectance over a wide region $\sim 50\,cm^{-1}$ to over $20{,}000\,cm^{-1}$ at 295 K to carry out a reliable Kramers-Kronig analysis. The results of such an analysis are shown in Fig. 2. Two ab-plane infrared-active TO phonons can be identified at 473.2 and $612.8\,cm^{-1}$ with $E \| a$-axis marked as A and B, respectively, in σ_1 shown in Fig. 2(a). While the $612.8\,cm^{-1}$ mode is also observed with $E \| b$-axis, the $473.2\,cm^{-1}$ mode is completely absent and a new mode appears at $325.2\,cm^{-1}$ marked as C in Fig. 2(b). It is perhaps not surprising that only three ab-plane

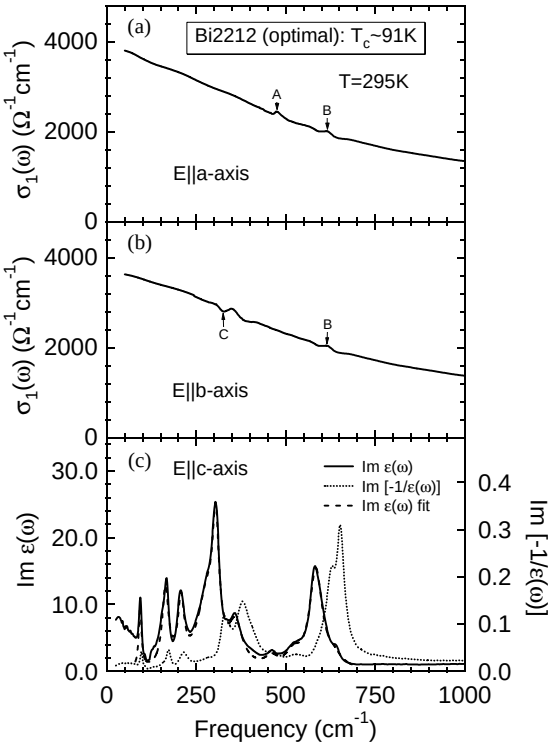

Fig. 2. Optical phonons in optimally doped Bi2212 single crystals at 295 K. (a) Two optical phonons at 473.2 and 612.8 cm^{-1} are observed in σ_1 with $E\|a$-axis in ab-plane. (b) Two optical phonons at 325.2 and 612.8 cm^{-1} are observed in σ_1 with $E\|b$-axis in ab-plane. (c) Ten optical TO phonons observed in Im $\varepsilon(\omega)$ with $E\|c$-axis in ac-plane with a fit with ten Lorentzians; ten corresponding optical LO phonons are observed in the loss function Im$[-1/\varepsilon(\omega)]$.

infrared-active modes are observed in σ_1 instead of $7E_u$ modes predicted by the D_{4h} space group. Many of these in-plane modes would be screened by the charge carriers in the ab-plane particularly those involving the vibrations within the CuO_2 planes. Therefore these three infrared-active in-plane modes at 325.2, 473.2 and 612.8 cm^{-1} are quite likely originated from in-plane oxygen vibrations in the BiO and SrO layers. The c-axis infrared-active phonons are shown in Fig. 2(c) at 295 K. It is better to examine the imaginary part of the dielectric function directly instead of plotting σ_1 for $E\|c$-axis. Ten c-axis infrared-active TO phonons can be identified in Im $\varepsilon(\omega)$ with the corresponding LO phonons derived from the loss function Im$[-1/\varepsilon(\omega)]$ given in bracket: 93.3 (96.4), 164.1 (171.6), 207.7 (213.4), 280.5 (283.5), 304.4 (327.8), 360.3 (378.6), 460.2 (463.5), 521.4 (527.1), 584.4 (628.7) and 625.1 (651.8) cm^{-1}. More c-axis infrared-active phonons are observed in the present work then the $6A_{2u}$ phonons predicted by the D_{4h} space group.

The observed strong ab-plane phonon anisotropy is quite surprising giving the small orthorhombic distortions in optimally doped Bi2212. The strong polarization dependence of the 325.2 and 473.2 cm^{-1} modes indicates that they might be quasi-one-dimensional oxygen vibrations along b- and a-axis, respectively, ab-plane phonon anisotropy in optimally doped Bi2212 is inconsistent with the simplified D_{4h} space group assignment. The other indication of the inadequacy of the D_{4h} space group assignment is the fact that ten infrared-active c-axis phonons have been observed in this work while the D_{4h} space group predicts only six. In fact, our conclusion is similar to the Raman study on Bi2212 by Liu et al. [3] where they have demonstrated that the large number of peaks of A_{1g} symmetry observed experimentally is inconsistent with the D_{4h} space group and have used an alternative analysis based on an orthorhombic cell to explain their data. However, Liu et al. [3] have chosen a centrosymmetric space group Bbmb [11] to describe the orthorhombic subcell. However, many of the infrared-active phonons have energies that are very close to that of the Raman-active modes measured by Liu et al. [3]. Based on this observation, we conclude that it is more reasonable to use the space group without centrosymmetry, i.e., A2aa [12] for Bi2212. A detailed group theory analysis is needed to account for all the observed infrared-active and Raman-active phonons in Bi2212.

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