Explanation of non-linear in-plane electrical resistivity of YBa$_2$Cu$_4$O$_8$: electron-phonon approach

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Abstract. The temperature-dependent in-plane normal state electrical resistivity of single crystal YBa$_2$Cu$_4$O$_8$ is theoretically analysed within the framework of classical electron-phonon i.e., Bloch-Gruneisen model of resistivity. The contributions to the resistivity due to the inherent acoustic phonons as well as high frequency optical phonons were first estimated. Estimated contribution to in-plane electrical resistivity by considering both phonons along with the zero limited resistivity, when subtracted from single crystal data infers a quadratic temperature dependence over most of the temperature range which is understood in terms of electron-electron inelastic scattering. The value of the electron-phonon coupling strength and of the Coulomb screening parameter obtained from the static dielectric function with the two-dimensional model and is in the strong coupling limit. As an application of the proposed model, the superconducting transition temperature $T_c$ is also estimated. Apart from phonons if we add charge density waves for pairing, we retrieve the experimental reported $T_c$ value.

1. Introduction

The pairing mechanism and electrical transport of high-$T_c$ cuprate superconductor’s remains elusive in spite of the fact that many models have been proposed since its discovery. The pairing symmetry in cuprate superconductors is an important and much debated issue [1]. Phonons are important in an ionic lattice such as YBa$_2$Cu$_3$O$_{6-}$, The Raman scattering of light have been employed to probe its phonon structure, four Raman modes of the double Cu(1)-O(1) chains assign the peaks to Cu(1) $A_g$ (250 cm$^{-1}$), O(1) $A_g$ (605 cm$^{-1}$), Cu(1) $B_{3g}$ (314 cm$^{-1}$) and O(1) $B_{2g}$ (228 cm$^{-1}$), in addition to the 5 $A_g$ phonons near 104, 153, 341, 438 and 500 cm$^{-1}$ [2]. A distinct feature of the normal state of high-$T_c$ superconductors is the linear increases in the resistivity over large temperature range [3-5]. In YBa$_2$Cu$_3$O$_7.6$ (1:2:3) a deviation from linearity was measured only for T$\geq$600 K due to loss of oxygen [3]. Both the in-plane and out-of-plane resistivities show a distinct change in behavior on cooling from high temperatures. The chain resistivity $\rho_{\text{chain}}(T)$, by contrast, obeys a $T^2$ law over the entire temperature range. The c-axis resistivity $\rho_c(T)$ is almost $T$ independent at high $T$ [6]. Here, we propose a model to explain the temperature dependent resistivity as arising from the scattering of carriers to both acoustic and optical phonons. Usually, the temperature dependence of resistivity reflects an overall electron-phonon
coupling strength. The electron-phonon coupling strength determines the superconducting $T_c$, hence temperature dependent behaviour of resistivity and superconducting $T_c$ is intimately related.

2. The model

The zero temperature-limited resistivity is expressed as [7]

$$\rho(0) = \frac{4\pi\tau^{-1}}{\omega_p^2}$$

(1)

Where $\omega_p$ is the plasma frequency and $\tau$ is relaxation time.

The temperature dependent part of the resistivity is [8]

$$\rho = \frac{3\pi}{h e^2 v_F^2} \int_0^{2k_F} \left| v(q) \right|^2 \left( \frac{1}{2k_F} \right)^4 q^3 dq.$$  

(2)

$v(q)$ being the Fourier transform of the potential associated with one lattice site and $S(q)$ denotes the structure factor and within the Debye model it takes the following form

$$\left| S(q) \right|^2 \approx \frac{k_BT}{M v_s^2} \left[ \exp\left( \frac{\hbar\omega_q}{k_BT} \right) - 1 \right] \left( 1 - \exp\left( -\frac{\hbar\omega_q}{k_BT} \right) \right)$$

(3)

yielding

$$\rho \approx \left( \frac{3}{h e^2 v_F^2} \right) \frac{k_BT}{M v_s^2} \left| v(q) \right|^2 \left[ \exp\left( \frac{\hbar\omega_q}{k_BT} \right) - 1 \right] \left( 1 - \exp\left( -\frac{\hbar\omega_q}{k_BT} \right) \right)$$

(4)

$v_s$ being the sound velocity. Equation (4) in terms of acoustic phonon contribution yields the Bloch-Gruneisen function of temperature dependence resistivity:

$$\rho_{ac}(T, \theta_D) = 4 A_{ac}(T/\theta_D)^4 \int_0^{\theta_D/T} x^5 (e^x - 1)^{-1} (1 - e^{-x})^{-1} \, dx.$$  

(5)

where, $x = \hbar\omega/k_BT$. $A_{ac}$ is being a constant of proportionality defined as

$$A_{ac} \equiv \frac{3\pi^2 e^2 k_B}{k_F^2 v_s^2 L \eta^2 M}$$

(6)

A model phonon spectrum consisting of two parts: an acoustic Debye branch characterized by the Debye temperature $\theta_D$ and an optical peak defined by the Einstein temperature $\theta_E$. If the Matthiessen rule is obeyed, the resistivity may be represented as a sum $\rho(T) = \rho_0 + \rho_{e-ph} (T)$, where $\rho_0$ is the residual resistivity that does not depend on temperature. On the other hand, in case of the Einstein type of phonon spectrum (an optical mode) $\rho_{op}(T)$ may be described as follows

$$\rho_{op}(T, \theta_D) = A_{op} \theta_E^2 T^{-1} \left[ \exp(\theta_E/T) - 1 \right]^{-1} \left[ 1 - \exp(-\theta_E/T) \right]^{-1}.$$  

(7)

$A_{op}$ is defined analogously to equation (6). Thus, the phonon resistivity can be conveniently modelled by clubbing both terms arose from acoustic and optical phonons

$$\rho_{e-ph}(T) = \rho_{ac}(T, \theta_D) + \rho_{op}(T, \theta_E)$$

(8)

We shall use the values of various physical parameters in next section to estimate the zero limited resistivity and temperature dependent contribution in high-$T_c$ YBa$_2$Cu$_3$O$_7$ superconductors.

3. Results and Discussion

While calculating the Debye and Einstein temperatures, we take $s = 10$ and the in plane Cu-O distance as 1.833 Å, yielding $\kappa = 16.84 \times 10^4$ gm s$^{-2}$ and $\eta = 1.91 \times 10^4$ gm s$^{-2}$. For most ionic crystals, the index number of the repulsive potential has been reported to be $s = 6 \sim 8$ [9]. However, for Copper oxides a reasonable value of the repulsive index is about 10 [10]. With these parameters the Debye frequency is
estimated as 42.36 meV (491.33 K) and is consistent with the specific heat measurement [11]. Further the optic phonon mode is obtained as $\omega_{LO} \simeq 61.1$ meV (708.76 K) and $\omega_{TO} \simeq 54.52$ meV (632.44 K). The calculated values of the LO/TO frequency are consistent with the measured values of the $A_{2u}$ optical phonons from the Raman spectra of YBa$_2$Cu$_4$O$_8$ superconductor’s [12, 2].

![Figure 1](https://example.com/figure1.png)

**Figure 1.** Variation of $\rho$ with temperature $T$ (K). Open circles represent the experimental data taken from Bucher et al. (1994) [15]. Inset of figure shows the variation of $\rho_{\text{diff}} \{ = \rho_{\text{exp}} - \rho_0 + \rho_{\text{e-ph}} \} (x \times 10^{-4} \Omega \text{cm})$ with $T^2$ ($10^4$ K$^2$).

In order to estimate the zero-limited resistivity, we use the plasma frequency $\omega_p (= 2.5$ eV) [13], deduced from the electronic energy band structure calculations. With the above model parameters, the zero temperature elastic scattering rates is obtained as $0.7 \times 10^{14}$ sec$^{-1}$. We further estimate the zero temperature mean free path, $L = v_F \tau \approx 18$ Å which is much smaller than the zero temperature coherence length of 41-45 Å [14]. A significantly enhanced mean free path is an indicative of metallic conduction as the product $k_F L (\sim 7.5)$ seems to be much larger than unity. Zero temperature limited resistivity ($\rho_0 = 1.6 \mu \Omega \text{cm}$) as deduced from elastic scattering rate and plasma frequency.

Figure 1 shows the results of temperature dependence of resistivity via the ordinary electron-phonon interaction from equation (8) with our choice of $\theta_D (= 491$ K) and $\theta_E (\omega_{TO} = 632$ K). The contributions of acoustic and optical phonons lies in CuO$_2$ planes and CuO chains towards resistivity are shown separately along with the total resistivity. It is inferred from the plot that $\rho_{ac}$ increases linearly, while to that $\rho_{op}$ increase exponentially with the increase in temperature, these observations shows that the more of acoustic phonons lies in the planes where the more of optical phonons lies in chains. Both the contributions are clubbed and the resultant resistivity is exponential at low temperatures, and nearly linear at high temperatures till room temperature.
Our numerical results on temperature dependence of resistivity of YBa$_2$Cu$_4$O$_8$ are also plotted in figure 1 along with the single crystal data [15]. It is noticed from the plot that the estimated $\rho$ is lower than the reported data from $T_c$ to near room temperature. The difference in between the measured $\rho$ and calculated $\rho_{\text{diff.}} = \rho_{\text{exp.}} - \left\{ \rho_0 + \rho_{\text{e-ph}} \left( = \rho_{\text{ac}} + \rho_{\text{op}} \right) \right\}$ in the temperature range 80 K to 300 K is plotted (see inset of figure 1). A quadratic temperature dependence of $\rho_{\text{diff.}}$ is depicted at low (~ 80 K) as well near to room temperature. The quadratic temperature contribution for resistivity is an indication of conventional electron-electron scattering. The additional term due to electron–electron contribution was required in understanding the resistivity behaviour, as extensive attempts to fit the data with residual resistivity and phonon resistivity were unsuccessful.

The phonon spectrum in view of inelastic neutron scattering measurements consists of two parts, the electron–phonon coupling strength is conveniently divided into two terms $\lambda_{\text{ac}}$ and $\lambda_{\text{op}}$, that are intimately related with Eliashberg function $\alpha^2 F(\omega)$. At high temperatures $\rho_{\text{ac(op)}} (T) \propto \lambda_{\text{ac(op)}}$ and hence it is appropriate to write $\lambda_{\text{ac}}/\lambda_{\text{op}} = A_{\text{ac}}/A_{\text{op}}$. We find the ratio $A_{\text{op}}/A_{\text{ac}}$ as 1.56 leading roughly $\lambda_{\text{ac}} \approx 0.45$, $\lambda_{\text{op}} \approx 0.7$ and $\lambda_{\text{ac}} + \lambda_{\text{op}} \approx 1.15$. Using above coupling constants we evaluated the transition temperature $T_c$ for Y-Ba$_2$Cu$_4$O$_8$ to be about 25 K; which is consistent with experimental data.

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