Model of C-Axis Resistivity of High-$T_c$ Cuprates

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Abstract

We propose a simple model which accounts for the major features and systematics of experiments on the $c$-axis resistivity, $\rho_c$, for La$_{2-x}$Sr$_x$CuO$_4$, YBa$_2$Cu$_3$O$_{6+x}$ and Bi$_2$Sr$_2$CaCu$_2$O$_8$. We argue that the $c$-axis resistivity can be separated into contributions from in-plane dephasing and the $c$-axis "barrier" scattering processes, with the low temperature semiconductor-like behavior of $\rho_c$ arising from the suppression of the in-plane density of states measured by in-plane magnetic Knight shift experiments. We report on predictions for $\rho_c$ in impurity-doped YBa$_2$Cu$_3$O$_{6+x}$ materials.
Although there is currently no consensus \[1\] as to the important mechanisms contributing to \(c\)-axis transport in high temperature superconductors, recent transport and optical experiments of \(\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_x\), \(\text{YBa}_2\text{Cu}_3\text{O}_{6+x}\), and \(\text{La}_{2-x}\text{Sr}_x\text{CuO}_4\) \[2\]–\[4\] reveal a number of key features that must be accounted for in any successful model of the interlayer charge dynamics in the layered cuprates: First, \(\rho_c(T)\) in \(\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8\) and underdoped \(\text{La}_{2-x}\text{Sr}_x\text{CuO}_4\) and \(\text{YBa}_2\text{Cu}_3\text{O}_{6+x}\) have a semiconductor-like temperature dependence \((d\rho_c/dT < 0)\) at low temperatures, and a linear-in-\(T\) dependence at high temperatures. The crossover temperature, \(T^\ast\), between these two regimes decreases with increased doping in \(\text{YBa}_2\text{Cu}_3\text{O}_{6+x}\) and \(\text{La}_{2-x}\text{Sr}_x\text{CuO}_4\). Importantly, \(c\)-axis optical measurements \[5\] show that the semiconductor-like resistivity “upturn” in underdoped \(\text{YBa}_2\text{Cu}_3\text{O}_{6+x}\) is actually associated with a uniform suppression of the optical conductivity below \(\sim 300 cm^{-1}\). These data suggest that the \(c\)-axis conductivity scales at low frequency with the Knight shift, which is proportional to the in-plane density of states: \(K_s \propto N(0)\). Second, both \(\text{La}_{2-x}\text{Sr}_x\text{CuO}_4\) and \(\text{YBa}_2\text{Cu}_3\text{O}_{6+x}\) exhibit a strongly doping-dependent mass anisotropy, and a possible crossover from quasi-2D to 3D transport behavior at high doping, that arises in part from doping-induced structural changes \[6\]–\[7\].

In this paper, we present a simple phenomenological model of the \(c\)-axis resistivity in the layered cuprates that describes the key elements of interlayer transport in the cuprates with reasonable parameters. Before examining the mechanisms contributing to \(c\)-axis transport in the cuprates, it is important to point out that experiment evidence suggests that, except perhaps for the overdoped cuprates, \(c\)-axis transport in high \(T_c\) superconductors is incoherent. For example, typical estimates of the \(c\)-axis scattering rate in \(\text{YBa}_2\text{Cu}_3\text{O}_{6+x}\) give \(1/\tau_c > 1000 cm^{-1}\) \[\frac{1}{\tau_c}\], while optical measurements indicate a \(c\)-axis plasma frequency of \(\omega_{p\perp} \sim 40 meV\) in fully oxygenated \(\text{YBa}_2\text{Cu}_3\text{O}_7\), and \(\omega_{p\perp} < 10 meV\) in underdoped \(\text{YBa}_2\text{Cu}_3\text{O}_{6+x}\) \[\frac{1}{\tau_c}\]. These values suggest that the \(c\)-axis mean free path is of order or less than the \(c\)-axis lattice spacing, i.e., \(c\)-axis conductivity in the cuprates is below the Ioffe-Regel limit, and hence \(c\)-axis transport is incoherent.

One important contribution to \(c\)-axis transport in the cuprates is expected to arise from
electron scattering in the “barrier” layer between CuO$_2$ “cells” (i.e., layers, bilayers, trilayers, etc.). For example, c-axis Raman scattering measurements provide evidence that carriers hopping between layers scatter from c-axis optical phonons associated with the barrier in YBa$_2$Cu$_3$O$_{6+x}$ [2], while Littlewood and Varma have pointed out the likelihood that static impurities in the barrier layer provide an important source of scattering for c-axis transport in the cuprates [1]. A phenomenological expression for this contribution to c-axis transport can be written as:

$$\sigma_c^{(1)} = N(0) \frac{e^2 d^2}{\hbar^2} t_{\perp}^2 \tau_c$$

(1)

where $d$ is the interlayer spacing, $N(0)$ is the in-plane density of states, $t_{\perp}$ is the interlayer coupling, and $\tau_c$ is the c-axis scattering time.

On the other hand, c-axis transport measurements of La$_{2-x}$Sr$_x$CuO$_4$ and Bi$_2$Sr$_2$CuO$_x$ yield $\rho_c \propto \rho_{ab}$ at high temperatures [4,8], suggesting that scattering or fluctuations in the planes may dominate c-axis transport in this regime. This contribution to c-axis transport can be written [9],

$$\sigma_c^{(2)} = N(0) \frac{e^2 d^2}{\hbar^2} t_1^2 \tau_{ab}$$

(2)

where $\tau_{ab}$ can be derived from the planar conductivity,

$$\sigma_{ab} = \frac{\omega_p^2}{L} \tau_{ab}$$

(3)

and the temperature-independent quantity, $t_1$, measures the effectiveness of planar scattering processes to c-axis transport.

Because Eqs.(1) and (2) describe independent physical processes, it seems natural to consider the corresponding tunneling and/or scattering mechanisms as additive in the resistivity. We are thus led to propose the following expression for $\rho_c$,

$$\rho_c = \frac{\hbar^2}{N(0)e^2d^2} \left( \frac{1}{t_{\perp}^2 \tau_{ab}} + \frac{1}{t_1^2 \tau_c} \right).$$

(4)

In the limit that one mechanism or the other is dominant, Eq.(1) yields the corresponding conductivity given in Eqs.(1) and (2). We now proceed to use Eq.(4) to analyze c-axis transport experiments.
We consider first the La$_{2-x}$Sr$_x$CuO$_4$ system. We obtain the temperature-dependent density of states $N(0)$, from the recent analysis by Barzykin, Pines and Thelen [10], who extract the temperature-dependent uniform susceptibility, $\chi_o(T)$, from Knight shift measurements and scaling arguments on this system; in deriving $N(0)$, we neglect Fermi liquid corrections, determining $N(0)$ from $\chi_o(T) = -\mu_B^2 N(0)$ where $\mu_B$ is the Bohr magneton. The density of states $N(0)$ obtained from the Knight shift data of Ohsugi et al [11] is shown in Fig. 1. We determine $\tau_{ab}$ by using Eq.(3) and optical measurements of $\omega_p\parallel$ [7]. An independent measure of $t_\perp$, the interlayer hopping amplitude, can be obtained from the c-axis plasma frequency, $\omega_{p\perp}$, measured in optical or penetration depth experiments [7]. This leaves us with a two-parameter fit to the data for each hole doping, these parameters being $t_1$ and $1/\tau_c$. Our results are given in Fig. 2 and Table I, and we comment on them briefly.

We first note that at each doping level, the high temperature behavior of $\rho_c$ is determined entirely by the planar conductivity, according to Eq.(2), so that $t_1$ is completely determined by $\rho_{ab}$. The values of $t_1$ obtained in this way are independent of hole concentration, within 10%. Secondly, both $t_\perp$ and $\tau_c$ are independent of temperature, and the barrier layer scattering contribution described by Eq.(1) dominates at sufficiently low temperatures. As might have been expected, $\tau_c$ is essentially independent of doping, while $t_\perp$, which increases with increasing hole concentration, displays a strong dependence on hole doping where $t_\perp \sim x^\alpha$ with $\alpha > 2$. According to Eq.(4), the crossover temperature $T^*$, which separates the $d\rho_c/dT < 0$ and $d\rho_c/dT > 0$ regimes, occurs when the two terms in the parenthesis of Eq.(4) are equal. After some simple algebra, we find that at $T^*$, we have

$$\frac{\rho_c(T^*)}{\rho_{ab}(T^*)} = \frac{\hbar^2}{N_{T^*}(0)e^2d^2}\left(\frac{2}{t_1^2\tau_{ab}}\right)/(\frac{4\pi}{\hbar^2\omega_{p\parallel}^2\tau_{ab}}) = \frac{\hbar^2\omega_{p\parallel}^2}{2\pi N_{T^*}(0)e^2d^2t_1^2}$$

where $N_{T^*}(0)$ is the density of states at $T=T^*$. Roughly, both $N_{T^*}(0)$ and $\omega_{p\parallel}$ increase with doping concentration, while all the other quantities on the right hand side of Eq.(5) are doping independent. It turns out that the anisotropy ratio $\rho_c/\rho_{ab}$ at the crossover temperature $T^*$ is nearly independent of hole doping for each individual cuprate. Thus for La$_{2-x}$Sr$_x$CuO$_4$, Nakamura et al [4] found $\rho_c/\rho_{ab} \sim 300$ at $T=T^*$, for doping levels of
We now apply the same method of data analysis to YBa$_2$Cu$_3$O$_{6+x}$ experiments. Our results are shown in Figs. 3 and 4, and Table I. In Fig. 3, we give our results for $N(0)$, obtained from the analysis by Ref. [13] of the Knight shift experiments of Ref. [12]. The nearly doping independent results for $\tau_c$ shown in Table I are taken from fits to optical and far infra-red experiments [3]. Again we see that $t_\parallel$ is nearly independent of hole concentration, while $t_\perp$ increases with hole doping as $t_\perp \sim x^\alpha$ where $\alpha > 2$. The anisotropy ratio at the crossover temperature $T^*$ remains almost doping independent. According to the data of Ref. [3], this ratio is $\rho_c/\rho_{ab} \sim 100$ at $T=T^*$ for different doping levels.

A further test of our model is provided by the $c$-axis resistivity measurements on Bi$_2$Sr$_2$CaCu$_2$O$_8$ shown in Fig. 5, which display the same qualitative dependence on temperature. Our theoretical results are obtained by deducing $N(0)$ from the Knight shift experiments of Walstedt et al [14], $\tau_{ab}$ from the measurements by Martin et al of $\rho_{ab}$ and $t_\perp$ from Ref. [7]. The agreement between our model calculation and experiment is again seen to be satisfactory. The parameters used in making the fit given in Table I.

It is instructive to compare the variations in $t_\parallel$ and $t_\perp$ on going from one system to another. The fact that $t_\parallel$ is the largest in YBa$_2$Cu$_3$O$_{6+x}$, somewhat smaller in La$_{2-x}$Sr$_x$CuO$_4$ and smallest in Bi$_2$Sr$_2$CaCu$_2$O$_8$ suggests that although independent of doping, the dephasing of the $ab$-plane enters $\rho_c$ in a way which is related to the interlayer (unit cell) distance in these cuprates. Another observation from Table I is the systematic behavior of the $c$-axis “barrier” scattering rate $1/\tau_c$: the scattering is strongest in YBa$_2$Cu$_3$O$_{6+x}$, which contains two apical oxygens per unit cell; weaker in La$_{2-x}$Sr$_x$CuO$_4$, which has one apical oxygen per unit cell; and significantly reduced in Bi$_2$Sr$_2$CaCu$_2$O$_8$, which does not contain any apical oxygens. Our result for $1/\tau_c$ is also consistent with the Drude fitted results from optical and Raman experiments for YBa$_2$Cu$_3$O$_{6+x}$ [34]. All these facts support the suggestion that the $c$-axis barrier scattering originates most likely from the $c$-axis apical oxygen phonons.

c-axis transport measurements on impurity-doped systems provide a direct test of our description of $\rho_c$ in Eq. (1). We consider two types of impurities: Zn and Co, both of which

$x = 0.10, x = 0.12, x = 0.15,$ and $x = 0.20.$
have been doped into YBa$_2$Cu$_3$O$_7$. Zn is known to go in as a planar substitute for Cu. To first order, it does not modify the planar density of states $N(0)$, or the in-plane scattering rate $1/\tau_{ab}$, nor will it influence $t_\perp$ and $\tau_c$. Therefore, we predict that for Zn doped YBa$_2$Cu$_3$O$_7$, the changes which take place in the $c$-axis transport will mirror the comparatively small increase, $\delta\rho_{ab} \propto n_{Zn}$, found for this system [13]. On the other hand, when Co is doped into YBa$_2$Cu$_3$O$_7$ up to a 2.5% doping level, it does not influence $T_c$ [16], and may plausibly be assumed to substitute for chain Cu atoms. It will therefore not affect $t_1$, $\tau_{ab}$, or $N(0)$, and we may expect $\sigma_c^{(2)}$, Eq.(2) to be unaffected by Co substitutes to this level. Nevertheless, we would expect that $t_\perp$, which is sensitive to the chains, will be reduced, thus increases the magnitude of the barrier scattering contribution to $\rho_c$, and we expect $\rho_c$ to have a temperature dependence somewhat similar to that of YBa$_2$Cu$_3$O$_7$: linear-in-$T$ for the whole temperature range, with the same slope but a larger residual resistivity at $T=0$.

In conclusion, we have presented a model for $c$-axis resistivity of high $T_c$ cuprates, in which both in-plane dephasing and the $c$-axis “barrier” scattering contribute to the $c$-axis resistivity. The behavior of the “barrier” scattering is consistent with that of the $c$-axis apical oxygen phonons. Our model fits quite well with the existing data on La$_{2-x}$Sr$_x$CuO$_4$, YBa$_2$Cu$_3$O$_{6+x}$ and Bi$_2$Sr$_2$CaCu$_2$O$_8$.

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FIGURES

FIG. 1. The planar density of states of La$_{2-x}$Sr$_x$CuO$_4$ obtained from the Knight shifts data of Ohsugi et al.\cite{11}, following the scaling analysis of Ref.\cite{10}.

FIG. 2. Calculated $\rho_c$ for La$_{2-x}$Sr$_x$CuO$_4$ at different doping levels (symbols), plotted against the experimental data of Nakamura et al.\cite{4} (solid lines).

FIG. 3. The planar density of states obtained from the analysis of Ref.\cite{13} for YBa$_2$Cu$_3$O$_{6+x}$, here we use $N(0)$ of Y$_{0.9}$Pr$_{0.1}$Ba$_2$Cu$_3$O$_7$ for YBa$_2$Cu$_3$O$_{6.88}$. The $N(0)$ for YBa$_2$Cu$_3$O$_{6.68}$ is an estimate from the scaling arguments given in Ref.\cite{13}.

FIG. 4. Calculated $\rho_c$ for YBa$_2$Cu$_3$O$_{6+x}$ at different doping levels (symbols), plotted against the experimental data of Takenaka et al.\cite{3} (solid lines).

FIG. 5. Calculated $\rho_c$ for Bi$_2$Sr$_2$CaCu$_2$O$_8$ (circles) in comparison with experimental data by different groups\cite{2}. $N(0)$ is obtained from the scaling analysis of the Knight shift measurement of Ref.\cite{14}.
|                  | $\omega_{pl}$ | $t_1$ | $1/\tau_{ab}$ | $t_\perp$ | $1/\tau_c$ | $(t^2_{1}/\tau_{ab})^{-1}$ [at 300K] | $(t^2_{\perp}/\tau_c)^{-1}$ |
|------------------|--------------|-------|---------------|----------|-----------|-------------------------------------|---------------------|
| YBa$_2$CuO$_{6.68}$ | 0.8 | 14.4 | $\sim 2kT$ | 7.3 | 100 | 0.25 | 1.88 |
| YBa$_2$CuO$_{6.78}$ | 1.0 | 14.1 | $\sim 2kT$ | 10.4 | 100 | 0.26 | 0.92 |
| YBa$_2$CuO$_{6.88}$ | 1.18 | 18 | $\sim 2kT$ | 16.7 | 100 | 0.16 | 0.36 |
| YBa$_2$CuO$_{6.93}$ | 1.4 | 16.6 | $\sim 2kT$ | 30-40 | 109 | 0.19 | 0.089 |
| La$_{1.90}$Sr$_{0.10}$CuO$_4$ | 0.44 | 3.37 | $\sim kT$ | 0.9 | 6.78 | 2.29 | 8.37 |
| La$_{1.88}$Sr$_{0.12}$CuO$_4$ | 0.57 | 2.78 | $\sim kT$ | 1.3 | 6.99 | 3.36 | 4.14 |
| La$_{1.85}$Sr$_{0.15}$CuO$_4$ | 0.7 | 3.11 | $\sim kT$ | 2.4 | 6.56 | 2.69 | 1.14 |
| La$_{1.80}$Sr$_{0.20}$CuO$_4$ | 0.87 | 3.01 | $\sim kT$ | 5.5 | 6.67 | 2.87 | 0.22 |
| Bi$_2$Sr$_2$CaCu$_2$O$_8$ | 1.25 | 0.88 | $\sim kT/2$ | 0.1 | 2.64 | 16.8 | 264 |
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Fig. 5
