Model of c-axis resistivity of high-T_c cuprates

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We propose a simple model which accounts for the major features and systematics of experiments on the c=axis resistivity, ρ_c for $La_{2-x}Sr_xCuO_4$, $YBa_2Cu_3O_{6+x}$, and $Bi_2Sr_2CaCu_2O_8$. 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 semiconductorlike behavior of ρ_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 ρ_c in impurity-doped $YBa_2Cu_3O_{6+x}$ 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 $Bi_2Sr_2CaCu_2O_x$, $YBa_2Cu_3O_{6+x}$, and $La_{2-x}Sr_xCuO_4$ (Refs. 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 $Bi_2Sr_2CaCu_2O_8$ and underdoped $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_{6+x}$ have a semiconductorlike temperature dependence ($d\rho_c/dT<0$) at low temperatures and a linear-in-T dependence at high temperatures. The crossover temperature T^* between these two regimes decreases with increased doping in $YBa_2Cu_3O_{6+x}$ and $La_{2-x}Sr_xCuO_4$. Importantly, c-axis optical measurements[5] show that the semiconductorlike resistivity ''upturn'' in underdoped $YBa_2Cu_3O_{6+x}$ is actually associated with a uniform suppression of the optical conductivity $\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 $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_{6+x}$ exhibit a strongly doping-dependent mass anisotropy, and a possible crossover from quasi-two-dimensional (quasi-2D) to 3D transport behavior at high doping, which 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. The microscopic justification of this phenomenology and its extension to the superconducting-state c-axis transport will be given in another publication. 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 $YBa_2Cu_3O_{6+x}$ give $1/\tau_c > 1000$ cm^{-1},[6] while optical measurements indicate a c-axis plasma frequency of $\omega_{p\perp} \sim 40$ meV in fully oxygenated $YBa_2Cu_3O_7$ and $\omega_{p\perp} < 10$ meV in underdoped $YBa_2Cu_3O_{6+x}$.[7] 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 $YBa_2Cu_3O_{6+x}$,[6] 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

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

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

On the other hand, c-axis transport measurements of $La_{2-x}Sr_xCuO_4$ and $Bi_2Sr_2CuO_x$ yield $\rho_c \propto \rho_{ab}$ at high temperatures,[4,9] 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[10]

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

where τ_{ab} can be derived from the planar conductivity

$$\sigma_{ab} = \frac{\omega_{p\parallel}^2}{4\pi}\tau_{ab} \tag{3}$$

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 ρ_c:

$$\rho_c = \frac{\hbar^2}{N(0)e^2 d^2}\left(\frac{1}{t_1^2\tau_{ab}} + \frac{1}{t_\perp^2 \tau_c}\right). \tag{4}$$

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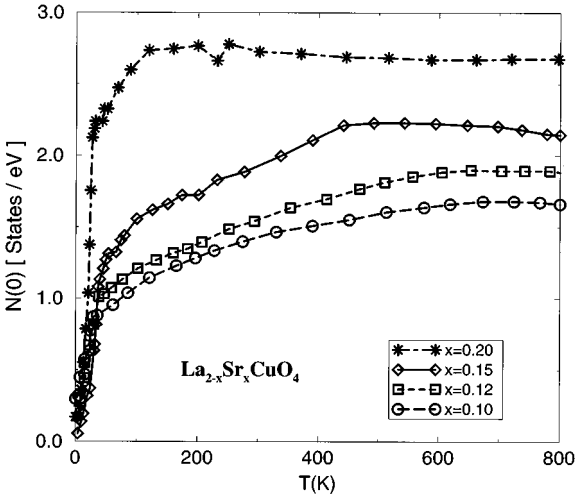

FIG. 1. Planar density of states $La_{2-x}Sr_xCuO_4$ obtained from the Knight shift data of Ohsugi *et al.* (Ref. 12), following the scaling analysis of Ref. 11.

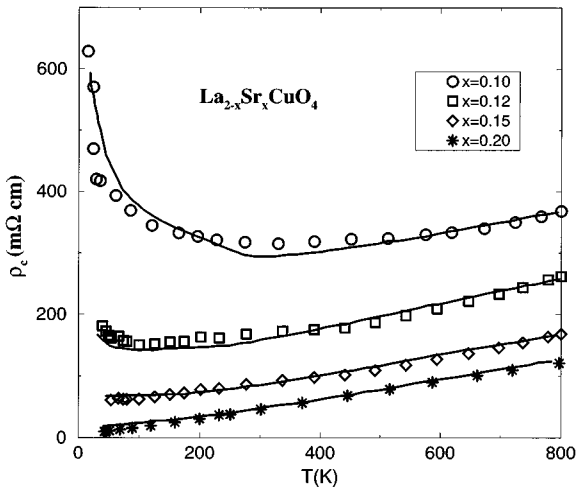

FIG. 2. Calculated ρ_c for $La_{2-x}Sr_xCuO_4$ at different doping levels (symbols), plotted against the experimental data of Nakamura and Uchida (Ref. 4) (solid lines).

In the limit that one mechanism or the other is dominant, Eq. (4) 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 $La_{2-x}Sr_xCuO_4$ system. We obtain the temperature-dependent density of states, $N(0)$, from the recent analysis by Barzykin *et al.*,[11] who extract the temperature-dependent uniform susceptibility $\chi_0(T)$ from Knight shift measurements and scaling arguments on this system; in deriving $N(0)$, we neglect Fermi liquid corrections, determining $N(0)$ from $\chi_0(T) = -\mu_B^2 N(0)$, where μ_B is the Bohr magneton. The density of states, $N(0)$, obtained from the Knight shift data of Ohsugi *et al.*[12] is shown in Fig. 1. We determine τ_{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 ρ_c is determined entirely by the planar conductivity, according to Eq. (2), so that t_1 is completely determined by ρ_{ab}. The values of t_1 obtained in this way are independent of hole concentration, within 10%. Second, both $t_\perp$ and τ_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, $t_\perp$ increases with increasing hole concentration and 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

$$\frac{\rho_c(T^*)}{\rho_{ab}(T^*)} = \frac{\hbar^2}{N_{T^*}(0)e^2d^2}\left(\frac{2}{t_1^2\tau_{ab}}\right) \Big/ \left(\frac{4\pi}{\omega_{p\parallel}^2\tau_{ab}}\right) = \frac{\hbar^2\omega_{p\parallel}^2}{2\pi N_{T^*}(0)e^2d^2t_1^2}, \tag{5}$$

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 ρ_c/ρ_{ab} at the crossover temperature T^* is nearly independent

TABLE I. Relevant numbers.

	$\omega_{p\parallel}$ (eV)	t_1 (meV)	$1/\tau_{ab}$ (meV)	$t_\perp$ (meV)	$1/\tau_c$ (meV)	$(t_1^2\tau_{ab})^{-1}$ [at 300 K] (meV^{-1})	$(t_\perp^2\tau_c)^{-1}$ (meV^{-1})
$YBa_2Cu_3O_{6.68}$	0.8	14.4	$\sim 2kT$	3.0	17	0.25	1.88
$YBa_2Cu_3O_{6.78}$	1.0	14.1	$\sim 2kT$	6.5	39	0.26	0.92
$YBa_2Cu_3O_{6.88}$	1.18	18	$\sim 2kT$	14	70	0.16	0.36
$YBa_2Cu_3O_{6.93}$	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	$\sim kT$	0.7	4.1	2.29	8.37
$La_{1.88}Sr_{0.12}CuO_4$	0.57	2.78	$\sim kT$	1.2	5.9	3.36	4.14
$La_{1.85}Sr_{0.15}CuO_4$	0.7	3.11	$\sim kT$	2.4	6.5	2.69	1.14
$La_{1.80}Sr_{0.20}CuO_4$	0.87	3.01	$\sim kT$	5.5	6.7	2.87	0.22
$Bi_2Sr_2CaCu_2O_8$	1.25	0.88	$\sim kT/2$	0.1	2.6	16.8	264

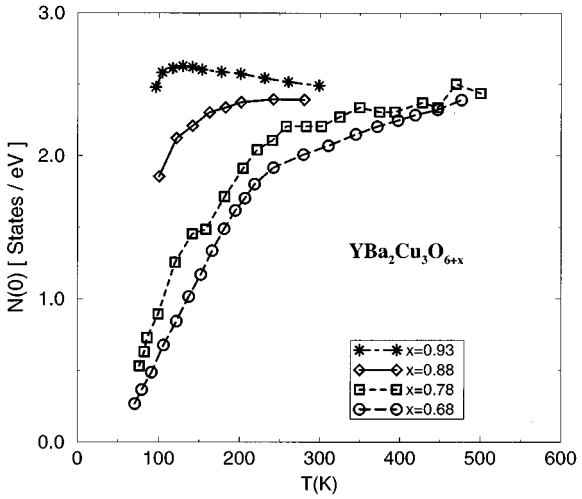

FIG. 3. Planar density of states obtained from the analysis of Ref. 13 for $YBa_2Cu_3O_{6+x}$; here, we use the $N(0)$ of $Y_{0.9}Pr_{0.1}Ba_2Cu_3O_7$ for $YBa_2Cu_3O_{6.88}$. The $N(0)$ for $YBa_2Cu_3O_{6.68}$ is an estimate from the scaling arguments given in Ref. 13.

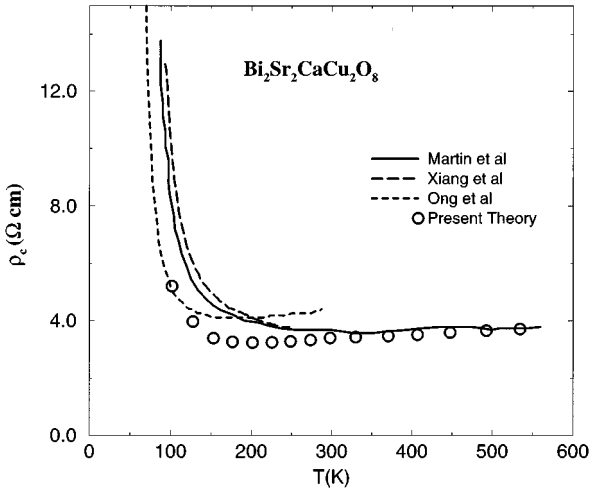

FIG. 5. Calculated ρ_c for $Bi_2Sr_2CaCu_2O_8$ (circles) in comparison with experimental data by different groups (Ref. 2). $N(0)$ is obtained from the scaling analysis of the Knight shift measurement of Ref. 15.

of hole doping for each individual cuprate. Thus for $La_{2-x}Sr_xCuO_4$, Nakamura and Uchida[4] found $\rho_c/\rho_{ab}\sim 300$ at $T=T^*$, for doping levels of $x=0.10$, 0.12, 0.15, and 0.20.

We now apply the same method of data analysis to $YBa_2Cu_3O_{6+x}$ 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. 14. Here $t_\perp$ shown in Table I is taken from Ref. 7. Again we see that t_1 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 $Bi_2Sr_2CaCu_2O_8$ shown in Fig. 5,

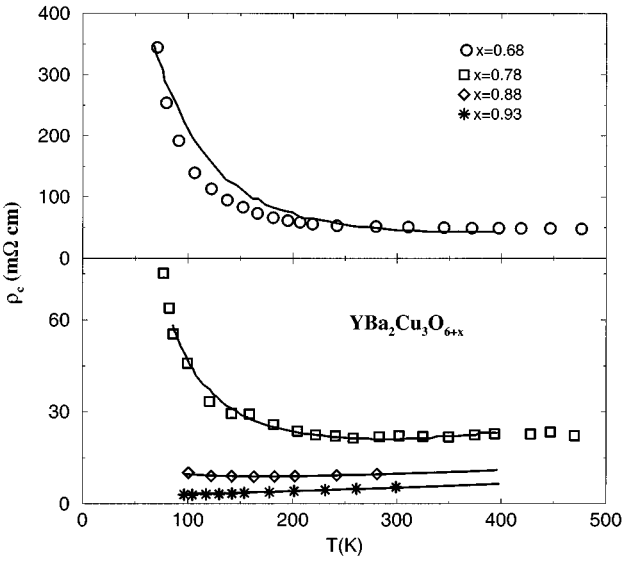

FIG. 4. Calculated ρ_c for $YBa_2Cu_3O_{6+x}$ at different doping levels (symbols), plotted against the experimental data of Takenaka *et al.* (Ref. 3) (solid lines).

which display the same quality dependence on temperature. Our theoretical results are obtained by deducing $N(0)$ from the Knight shift experiments of Walstedt *et al.*,[15] τ_{ab} from the measurements by Martin *et al.*[2] of ρ_{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 are given in Table I.

It is instructive to compare the variations in t_1 and $t_\perp$ on going from one system to another. The fact that t_1 is the largest in $YBa_2Cu_3O_{6+x}$, somewhat smaller in $La_{2-x}Sr_xCuO_4$, and smallest in $Bi_2Sr_2CaCu_2O_8$ suggests that, although independent of doping, the dephasing of the ab plane enters ρ_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 $YBa_2Cu_3O_{6+x}$, weaker in $La_{2-x}Sr_xCuO_4$ and significantly reduced in $Bi_2Sr_2CaCu_2O_8$. Also, our result for $1/\tau_c$ is consistent with the Drude-fitted results from optical and Raman experiments for $YBa_2Cu_3O_{6+x}$.[6,7] These suggest that $1/\tau_c$ may be due to the intrinsic disorder within the barriers layer. The Cu-O chain structure in the $YBa_2Cu_3O_{6+x}$ system may be a candidate of such intrinsic disorder, not only in the possible disorder in the chain, but also in the band structure mismatch between the chain and the plane bands.[8] This intrinsic disorder may also come from the Sr doping which goes to the barrier layer in $La_{2-x}Sr_xCuO_4$. For $Bi_2Sr_2CaCu_2O_8$, the c-axis is presumably ordered due to the lack of chains in its structure.

c-axis transport measurements on impurity-doped systems provide a direct test of our description of ρ_c in Eq. (4). We consider two types of impurities: Zn and Co, both of which have been doped into $YBa_2Cu_3O_7$. 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 τ_c. Therefore we predict that for Zn-doped $YBa_2Cu_3O_7$ 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.[16] On the other

hand, when Co is doped into $YBa_2Cu_3O_7$ up to a 2.5% doping level, it does not influence T_c very much[17] and may plausibly be assumed to substitute for chain Cu atoms.[18] It will therefore not affect t_1, τ_{ab}, or $N(0)$, and we may expect $\sigma_c^{(2)}$, Eq. (2), to be unaffected by Co substitutes to this doping level. Nevertheless, we would expect that $t_\perp$, which is sensitive to the chains, will be reduced, thus increasing the magnitude of the barrier scattering contribution to ρ_c, and we expect ρ_c to have a temperature dependence somewhat similar to that of $YBa_2Cu_3O_7$: linear in T for the whole temperature range, with the same slope, but a larger residual resistivity at $T=0$.

A fundamental question concerns the relationship between the semiconductorlike c-axis resistivity and the metallic in-plane resistivity in underdoped cuprate materials. Fits to the c-axis resistivities of different cuprates using the phenomenological description in Eq. (4) show that the low-temperature semiconductorlike upturn in ρ_c can be accounted for by the suppression of the planar density of states at low T, as determined from Knight shift data (i.e., spin pseudogap formation). While its origin is not clear at present, the pseudogap has been proposed by Ito *et al.*[19] and Bucher *et al.*[20] to also account for the deviation of $\rho_a(T)$ from linearity at T^* in $YBa_2Cu_3O_{6.6}$ and $YBa_2Cu_4O_8$. In our quantitative analysis, by assuming the quasiparticle nature of the planar spins, we derive density of states from the Knight shift data. This hypothesis is supported by the observation of Loram *et al.*,[21] who find the similar density of states from the specific heat measurement. Furthermore, the fact that the c-axis resistivity, as another charge response, fits well with Knight-shift-derived density of states gives further support to this initial hypothesis.

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. Our model fits quite well with the existing data on $La_{2-x}Sr_xCuO_4$, $YBa_2Cu_3O_{6+x}$, and $Bi_2Sr_2CaCu_2O_8$.

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