Temperature dependence of the c-axis resistivity of high-T_c layered oxides

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Electrical transport along the c axis of high-T_c layered oxides is pictured as a coherent interplanar tunneling between neighboring layers blocked by repeated intraplanar incoherent scatterings. This gives the same temperature dependence for the c-axis resistivity as that for the in-plane resistivity. Additional temperature dependence can arise from the temperature-dependent renormalization of the tunneling matrix element by an ohmic coupling to adiabatic phonons because of the large effective electron mass along the c axis. Our calculation is consistent with recent experimental results on single crystals, and makes some definite predictions that can be put to test.

The anisotropy of the temperature dependence of the normal-state electrical resistivity of high-T_c layered oxides is not understood at present, even at a qualitative level.[1] This is due partly to the disagreement among the different experimental groups as to the temperature dependence of the resistivity along the c axis. Thus, while there is a general agreement that the in-plane resistivity ρ_{ab} is metallic and grows linearly with temperature[1-7]—right from T_c upwards to the highest temperatures of measurement—the out-of-plane resistivity ρ_c has been reported variously to have a nonmetallic,[2-4] a metallic,[5,6] or a mixed[7] temperature dependence. More specifically, a nonmetallic power-law temperature dependence $\rho_c(T) \propto T^{-\alpha}$, with $0.5 < \alpha < 1$, has been reported by Martin *et al.*[4] on their highly anisotropic single crystals of the Bi 2:2:0:1 series of compounds (with T_c as low as 7 K, which is very much smaller than the transport Debye temperature). This is to be contrasted with the metallic behavior, $\rho_c(T) \propto T$ in single crystals of Y 1:2:3 as reported by Iye *et al.*[5] A mixed behavior of the form $\rho_c(T) = A/T + BT$ has been found by Hagen *et al.*[7] from their resistivity measurements on single crystals of Y 1:2:3 and is strongly supported by the Anderson-Zou mechanism.[8] One of the many questions now being asked is whether we are observing here the intrinsic c-axis transport at all—the high degree of anisotropy ($\rho_c/\rho_{ab} \gg 1$) makes it entirely possible for any measurement of the c-axis resistivity to pick up an in-plane component of the resistivity tensor. This may be externally due to a misalignment of contacts, or internally due to the randomly distributed defects, or "shorts," providing easy conduction paths between the ab planes.[3] However, the very recent measurements of Friedmann *et al.*[6] on twin-free single crystals of Y 1:2:3 show linear temperature dependence of resistivities ρ_a, ρ_b, and ρ_c along all the three orthorhombic axes. Their samples are claimed to have the lowest resistivities reported so far and may thus approximate well the intrinsic behavior. (For our purpose, the relatively small anisotropy in the ab plane is not important and we will just consider ρ_{ab}, the average of ρ_a and ρ_b).

Given this rather conflicting evidence and, indeed motivated by it, we propose in this work a general mechanism that intrinsically gives $\rho_c \propto \rho_{ab}$ and, therefore, the same metallic T-linear temperature dependence for ρ_c as is known for ρ_{ab}. In our model for electrical transport, the in-plane electron dynamics is taken to be bandlike, characterized by a Boltzmann-like mean free path, or equivalently a mean free lifetime τ between successive scatterings that are assumed inelastic and, therefore, break the quantum phase coherence. It is not necessary for us to assume any detailed model for these incoherent scatterings. All we need to say is that the temperature dependence of the in-plane resistivity comes entirely from that of τ via the Drude relation $\rho_{ab} = m_{ab}^*/ne^2\tau$, where m_{ab}^* is the in-plane effective mass. Thus, for instance, if the in-plane dynamics corresponds to that of a two-dimensional correlated electron system, modeled semiphenomenologically as a marginal Fermi liquid, then $1/\tau$ will be proportional to the imaginary part of the retarded self-energy of the electrons which in turn is proportional to temperature.[9] The crucial point of our model is that these incoherent in-plane scattering events interrupt and, therefore, block the coherent tunneling of the electron to the neighboring planes under the influence of the tunneling matrix element t_c, much the same way as the repeated "measurements" block the quantum evolution due to wave-function collapse.[10] This blocking is manifested quantitatively in the modification of t_c to $t_c^2\tau/\hbar \ll t_c$ for $t_c\tau/\hbar \ll 1$. The latter inequality implies that a large number of in-plane scatterings takes place before an interplanar tunneling occurs. This translates simply as large anisotropy, $\rho_c/\rho_{ab} \gg 1$, which will be assumed throughout. Under this condition, the successive interplanar tunneling events get uncorrelated and it is , therefore, sufficient to consider tunneling between just two

neighboring planes, labeled α and β, say.

Thus, our model Hamiltonian is (in obvious notation) $H=H_0+H'$, with

$$H_0=\sum_{k,\sigma}\varepsilon_k\alpha^\dagger_{k\sigma}\alpha_{k\alpha}+\sum_{k,\sigma}\varepsilon_k\beta^\dagger_{k\sigma}\beta_{k\sigma}+t_c\sum_k(\beta^\dagger_{k\sigma}\alpha_{k\sigma}+\text{H.c.})$$
$$\equiv H_\alpha+H_\beta+H_{\alpha\beta}\ , \tag{1}$$

where H' is the unspecified in-plane inelastic scattering term leading to the finite lifetime τ for transport of the ab planes. The effect of the "blocking" of the coherent interplanar tunneling due to repeated in-plane incoherent scatterings can be calculated straightforwardly following the treatment due to Simonius.[10] Thus, consider the time (t) evolution of an initial state $|\alpha,k_0\sigma\rangle$ of an electron lying in the plane "α," of wave vector k_0 and spin projection σ, under the tunneling Hamiltonian $H_{\alpha\beta}$, interrupted by the n-successive in-plane scattering: $|\alpha,k_0\sigma\rangle\rightarrow|\alpha,k_1\sigma\rangle\rightarrow\cdots\rightarrow|\alpha,k_n\sigma\rangle$, caused by H'. Let $\tau_1,\tau_2,\ldots,\tau_n$ be the corresponding time intervals between these n-successive scatterings, with the total time $\sum_i\tau_i=t$. The survival probability $P_{\alpha\alpha}$ for the electron to persist in the same plane "α" is now given by[10]

$$P_{\alpha\alpha}=\prod_{i=1}^{n}\left|\langle\alpha,k_{i\sigma}|e^{-iH}\alpha\beta^{\tau_i/\hbar}|\alpha,k_i\sigma\rangle\right|^2$$
$$\simeq\exp\left[-\frac{2t_c^2\tau}{\hbar^2}t\right],\quad\text{for } n\equiv t/\tau\gg1\ , \tag{2}$$

where we have assumed τ_i's to have the usual Poisson distribution with mean τ. From the in-plane survival probability given by Eq. (2), we can read off the rate of interplanar transition $\gamma_{\alpha\beta}$ as

$$\gamma_{\alpha\beta}=\left[\frac{2t_c^2\tau}{\hbar^2}\right]. \tag{3}$$

With $\gamma_{\alpha\beta}$ as the basic interplanar transition rate, we can now proceed to calculate the transport coefficient along the c axis. Let an external electric field of magnitude E be applied perpendicular to our pair of ab planes. This will generate a chemical-potential difference $\Delta\mu=edE$, where d is the distance between the two planes. This will expose a number of $\Delta\mu g$ of unoccupied states per unit area into which the electrons are free to make interplanar transitions. Here g is the density of states per unit area of the planes (counting both spins) and we have assumed a two-dimensional degenerate quasiparticle picture. The net interplanar current density will then be given by

$$j=e(\Delta\mu g)\gamma_{\alpha\beta}\ . \tag{4}$$

Thus we get the c-axis resistivity

$$\rho_c\equiv(E/j)=\left[\frac{\hbar^2}{2e^2dgt_c^2\tau}\right]. \tag{5}$$

The corresponding anisotropy ratio can now be written as

$$\rho_c/\rho_{ab}=4\left[\frac{a}{d}\right]^2\left[\frac{t_{ab}}{t_c}\right]^2\delta\ . \tag{6}$$

Here "a" is the in-plane lattice constant and δ is the number of change carriers per site in the plane. Also t_{ab} is the in-plane transfer matrix element. In arriving at Eq. (6) we have expressed τ in terms of ρ_{ab} via $\rho_{ab}=(m^*_{ab}/ne^2\tau)$, and reexpressed m^*_{ab}, as also the density of states g in terms of the in-plane bandwidth $=8t_{ab}$. Finally, the carrier concentration n is related to δ via $\delta=(nda^2)$.

Equation (6) is our main result. It predicts intrinsically the same temperature dependence for ρ_c as for ρ_{ab}. It also predicts a linear dependence of the anisotropy ratio on the carrier concentration δ. This is a verifiable feature. For the simple case of La 2:1:4 type systems we can identify δ with the hole concentration due to doping as, e.g., in $La_2CuO_{4-\delta}$. The ratio (t_{ab}/t_c) is essentially the effective mass ratio and can be estimated from the anisotropy of the London penetration depths (λ) via the anisotropic Ginzburg-Landau phenomenology, i.e., $(\lambda_c/\lambda_{ab})^2=(m_{ab}/m_c)$. Here λ_c and λ_{ab} correspond, respectively, to the magnetic fields along the c axis and the ab plane. Thus, for $(t_{ab}/t_c)=25$ to 100, $(a/d)\simeq0.5$, and typically $\delta\simeq0.1$, we get the anisotropy ratio $\rho_c/\rho_{ab}\simeq10^2$ to 10^3. We can expect much higher anisotropy for the Bi series because of presumably much larger (t_{ab}/t_c) ratio.

We would like to point out that additional power-law temperature dependence of ρ_c can come from the temperature dependence of the effective tunneling matrix element t_c itself due to its renormalization by the coupling of the slow interplanar electron tunneling to some adiabatic bosonic degrees of freedom as discussed by Kondo[11] in the context of the muon (heavy-electron) motion in metals. (Indeed, the electronic effective mass along the c axis here is comparable to that of muon.) In the present case we can reasonably identify the bosonic degrees of freedom with the acoustic phonons along the c axis. Such one-dimensional acoustic phonons can provide the necessary, indeed "ohmic" coupling in our case.[12] This would give an adiabatic modification of the tunneling matrix element $t_c\rightarrow\tilde{t}_c$ given by[12]

$$\tilde{t}_c=t_c\left[\frac{k_BT}{\hbar w_c}\right]^\alpha, \tag{7}$$

with

$$\alpha=\left[\frac{d^3\Lambda^2}{2\pi\hbar}\frac{1}{MC_s^3}\right].$$

Here w_c is an upper cutoff frequency ($\sim$ the Debye frequency), C_s is the acoustic phonon speed along the c axis, M is the unit-cell mass, and Λ is the deformation potential relevant to the electron phonon coupling. For a deformation potential of 0.5 eV Å^{-1} and $C_s\sim5\times10^5$ cm s^{-1}, α is of the order of unity. It is, however, not possible at the moment to estimate the exponent α accurately enough. It is believed, however, that in these materials

the electron-phonon coupling is rather weak and the α is expected to be small. It is clear, however, that this effect can qualitatively change the temperature dependence of ρ_c.

At this point we would like to note that recently Kumar *et al.*[13] have considered a model for anisotropic transport that involves scattering events of the type $|\alpha,k\sigma| \rightarrow |\beta,k'\sigma|$, i.e., the scattering not only randomizes momenta parallel to the *ab* plane but also causes interplanar transfers. This gave $\rho_c \propto 1/\rho_{ab}$. This mechanism is entirely different from the blocking of coherent tunneling considered in the present work. Also, both these mechanisms can operate simultaneously and can lead intrinsically to the mixed temperature dependence of the kind observed by Hagen *et al.*[7]

We will now comment on two finer points of our results. The first is the carrier concentration independence of $\rho_c(T)$ given by our Eq. (5). This is a direct consequence of our assumption of constant density of states (for the *two-dimensional* sheets) taken in conjunction with our mechanism of transport along the c axis. In the case of the usual Boltzmann transport in metals (as in the *in-plane* transport in our case) involving *hopping in the momentum space,* the carrier concentration enters indirectly through the (Fermi) velocity. It is not that *all* the electrons are involved in transport, but that all the electrons determine the (Fermi) velocity of those few that are. In the present case, the c-axis transport between the sheets involves tunneling *(real-space hopping)* between the states at the chemical potentials of the two sheets α and β, offset by the applied electric field as given by our Eq. (4). Here only the density of states at the chemical potential enters, and we have taken it to be constant because of two dimensionality. A systematic experimental study of concentration (in)dependence of ρ_c is called for.

The other point concerns the zero-temperature intercept of the experimental T-linear $\rho_c(t)$.[6] This is clearly an effect of disorder, which, although expected to be small for these single-crystal untwinned samples, can have considerable effects on ρ_c because of the smallness of the interplanar matrix element t_c. This effect can be included approximately by reinterpreting our Eq. (3) physically in a manner analogous to Eq. (38) of Kondo.[11] Thus, $\hbar/\tau$ in our Eq. (3) is the homogeneous level broadening due to intraplanar scatterings. In the presence of disorder, we should expect, in the zeroth approximation, an additional inhomogeneous level spread Δ which is temperature independent, and thus $\hbar/\tau$ is replaced by $\hbar/\tau+\Delta$. On substituting in Eq. (5) this gives us a zero-temperature intercept.

It may appear at first sight that the disorder Δ will affect the in-plane resistivity ρ_{ab} in the same proportion as it affects ρ_c through the above replacement of $\hbar/\tau$ by $\hbar/\tau+\Delta$. That this is *not* so and, indeed, that disorder affects ρ_{ab} *qualitatively* differently can be clarified by the following consideration. As we have argued above, the interplanar tunneling between the states $|\alpha,k\rangle$ and $|\beta,k\rangle$, where α and β label the nearest-neighboring planes, proceeds via the relatively small tunneling matrix element t_c and the effect of disorder is to broaden out inhomogeneously the density of states—it makes the matching of the energies of the two states $|\alpha,k\rangle$ and $|\beta,k\rangle$ having same k less favorable. In the case of the intraplanar conduction, the static disorder acts primarily as a mechanism of elastic scattering, $|\alpha,k\rangle \rightarrow |\alpha,k'\rangle$ say, and contributes an elastic relaxation time τ_e given by the Golden Rule as $1/\tau_e = (2\pi/\hbar) \times$ (the density of states at the the Fermi level) $\times$ (the *square* of the matrix element). The modification of the density of states at the Fermi level by the static disorder can be important only if the unperturbed density of states has a sharp structure at the Fermi level. Thus, disorder enters ρ_c and ρ_{ab} qualitatively differently. At the very least, Δ enters linearly for ρ_c in terms of $\hbar/\tau+\Delta$, while it is expected to enter quadratically for ρ_{ab} in terms of the matrix-element squared.

The slight upward turn of $\rho_c(T)$ at lower temperatures close to T_c can be attributed to the effect represented by our Eq. (7), though a weak-localization effect cannot be ruled out.

In conclusion we have presented a mechanism for the anisotropy of the temperature dependence of resistivity in the layered oxides involving blocking of coherent interplanar tunneling by the incoherent in-plane scattering. This gives intrinsically $\rho_c \propto \rho_{ab}$. The ratio $\rho_c/\rho_{ab} \propto \delta$, which can be and should be tested experimentally. Additional power-law temperature dependence may arise from the renormalization of the tunneling matrix elements due to ohmic coupling to adiabatic phonons. This mechanism, taken in conjunction with the one proposed recently by Kumar *et al.*, can give intrinsically a mixed temperature dependence of the kind observed by Hagen *et al.*[7] Finally, we believe that similar consideration should apply to other anisotropic layered systems; notable amongst them is graphite.[14,15]

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