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Metallic ground state of CuO chains in high-temperature superconductors

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We report on the metallic ground state of the CuO chains in $YBa_2Cu_4O_8$. The resistivities along the a and b directions have been determined for temperatures up to 900 K. Assuming a model of two shunted conduction channels along the b direction, representing the chain and plane resistivity, the resistivity of the chain ρ_{chain} has been calculated. Below 300 K, $\rho_{\text{chain}} \propto T^2$ and approaches a $T^{4/3}$ temperature dependence above 500 K. At least above T_c, two different kinds of free carriers exist simultaneously: highly correlated charge carriers inside the CuO_2 plane and itinerant electrons along the CuO chain.

Since the discovery[1] of high-temperature superconductors (HTSC) some years ago all kinds of experimental techniques have been applied in order to unravel the fundamental ingredients responsible for the high transition temperature T_c. The emerging results have been interpreted in terms of non-Fermi-liquid physics, near antiferromagnetic Fermi liquids, marginal Fermi liquids, induced superconductivity, and others.[2,3] Some physical quantities are consistent with the model of a Fermi liquid whereas others favored an explanation in terms of a non-Fermi-liquid approach.

All of the HTSC's comprise layered structures of CuO_2 planes and various layers in between like CuO chains, HgO layers, etc. Superconductivity is believed to be caused within the CuO_2 layers with the proximity effect generating superconductivity for the direction perpendicular to the CuO_2 plane. Most experimental results have been interpreted on the basis of being due mainly to the response of the CuO_2 plane. However should the other building blocks, e.g., the CuO chains, be metallic a more subtle analysis is required. Especially thermodynamical and spectroscopic measurements on polycrystalline or untwinned samples have to distinguish between plane and nonplane response. Indeed we corroborate in this paper that the double CuO chains of $YBa_2Cu_4O_8$ have a metallic ground state.

$YBa_2Cu_4O_8$ (1:2:4) is a genuinely untwinned, underdoped HTSC with the same structure as $YBa_2Cu_3O_7$ (1:2:3) but with the single CuO chain along the b axis replaced by a double CuO chain. In a previous paper[4] we focused on the CuO_2 plane of 1:2:4 and showed that the charge carriers are highly correlated with the dynamical spin susceptibility. The spin-gap behavior found by nuclear quadrupole resonance (NQR) and neutron-scattering experiments has been shown also to be manifest in the charge (transport) behavior inside the CuO_2 plane, i.e., the resistivity along the a direction. A puzzle has been the charge transport along the b direction of 1:2:4 consisting of CuO_2 plane and CuO chain conduction channels: there was no signature of the opening of the spin gap within the temperature dependence of ρ_b although the CuO_2 plane is involved in the charge transport along the b direction. Here we address this issue and will provide insight into the electronic structure of HTSC's corroborating the simultaneous existence of two different kinds of free carriers: highly correlated carriers inside the CuO_2 plane and weakly antiferromagnetically correlated itinerant carriers along the CuO chain.

Untwinned single crystals have been grown by a high-pressure flux method as described thoroughly by Karpinski *et al.*[5] Gold pads were sputter deposited along the crystallographic axes and thin gold wires had been attached on the pads by using gold epoxy. The contact resistances were in the order of 1 Ω.

The resistivity of $YBa_2Cu_4O_8$ has been measured on polycrystalline samples and thin films. Kapitulnik and Char[6] measured the ab-plane resistivity of a thin film 1:2:4 and have argued that the resistivity could be understood by means of a Bloch-Grüneisen (BG) theory assuming an effective transport Debye temperature Θ_D^{tr} which is about two times the thermodynamic Θ_D^{thermo}. They assumed that due to the strong anisotropy only longitudinal acoustic modes interact with the electrons preventing an averaging of the transverse and longitudinal sound velocities as in the thermodynamic Θ_D^{thermo}. Martin *et al.*[7] have measured the ab-plane resistivity of a thin film of 1:2:4 up to 600 K. In contrast to 1:2:3 they found a nonlinear temperature dependence which they also fitted with BG assuming an effective transport Debye temperature $\Theta_D^* \approx 500$ K. Triscone *et al.*[8] have reported transport data on polycrystalline 1:2:4 and were able to fit the resistivity with a BG function assuming an Einstein phonon distribution with the Einstein temperature $\Theta_E \approx 310$ K. All the measurements mentioned above have concluded BG-like transport *within* the ab plane. Our single-crystal measurements have revealed a more detailed situation: the resistivity along the a axis, ρ_a, which represents the conduction inside the CuO_2 plane correlates with the spin dynamics rather than with a phonon-dominated BG theory. But ρ_b, constituted by the plane and the chain response, was indeed consistent with a BG formalism; however, a very high $\Theta_D^{\text{tr}} \approx 800$ K was needed and, most puzzling, the spin-gap behavior has not been evident in spite of the plane channel contributing to the conductivity.

In Fig. 1(a), the resistivity of a single-crystal 1:2:4 is shown for $I \| a$ and $I \| b$, respectively. ρ_a reflects the opening of the spin gap at the temperature $T^* \approx 160$ K whereas ρ_b reveals the classical curvature of the BG theory. However, rather than exploiting the BG formula for the overall resistivity in the b direction[4] one could decompose the conduction channel along the b direction into two shunted conduction channels pertaining to chain, ρ_{chain}, and plane,

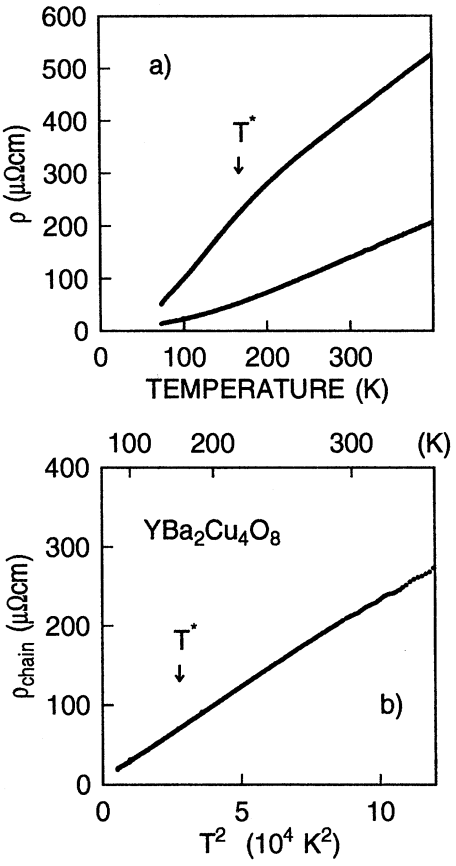

FIG. 1. (a) Resistivity of single-crystal $YBa_2Cu_4O_8$ for the a and b directions (ρ_a: upper curve; ρ_b: lower curve). ρ_a reflects the conductivity inside the CuO_2 plane; ρ_b represents the conduction along the double chain and CuO_2 plane. T^* denotes the opening of the spin gap above T_c. (b) Resistivity of the CuO chain alone as calculated with Eq. (1). The T^2 behavior levels off above 300 K. No signature of the opening of the spin gap is seen for the charge transport along the chain.

respectively. The plane contribution, ρ_{plane}, is represented by the resistivity along the a direction, i.e., $\rho_{\text{plane}}=\rho_a$. The resistivity along the chain can then be calculated by

$$\frac{1}{\rho_{\text{chain}}}=\frac{1}{\rho_b}-\frac{1}{\rho_a}. \tag{1}$$

From the data of ρ_a and ρ_b it is not at all predictable what should be expected for the calculated ρ_{chain}. The result is depicted in Fig. 1(b) on a square scale for the temperature. We found a T^2 behavior for the CuO chain for a temperature up to 300 K with a leveling off above. The opening of the spin gap at T^* has no influence for the transport inside the chain discarding a correlation of the spin dynamics of the CuO_2 planes across the in-between layers as the spin gap opens. The modeling of ρ_{chain} with

$$\rho_{\text{chain}}=\rho_0+AT^2 \tag{2}$$

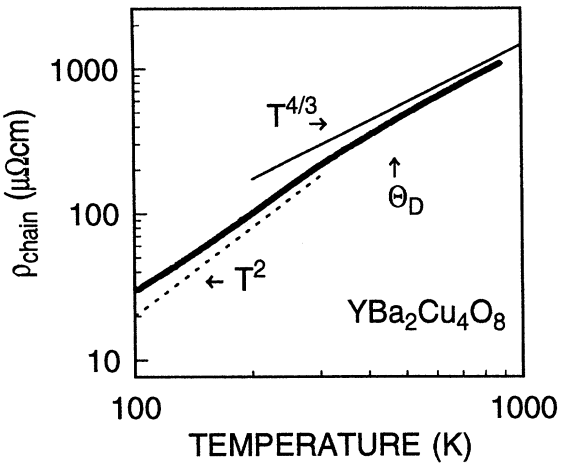

FIG. 2. Log-log plot of the resistivity of the CuO chain, ρ_{chain}, clarifying the high-temperature behavior above the Debye temperature Θ_D.

gives the parameter $\rho_0\sim 10\ \mu\Omega$ and $A=2.3\times 10^{-3}$ $\mu\Omega$ cm/K^2. The low residual resistivity ρ_0 points to the good sample quality with minor disorder within the quasi-one-dimensional CuO chain.[9] From the point of view of two shunted conduction channels for the resistivity along the b direction, the genuine temperature dependences of the chain ($\rho\propto T^2$) and the spin-gap behavior within ρ_a, combine to a pseudo-BG form of ρ_b as seen in thin films and polycrystalline material and resolves the puzzle why the opening of the spin gap is not seen within the resistivity of ρ_b.

A temperature dependence $\rho\propto T^2$ has been predicted for two- and three-dimensional electron-electron (ee) scattering. A one-dimensional system with ee scattering should expose $\rho\propto T^2$ below a switch-over temperature T_0 and $\rho\propto T$ above T_0, whereby T_0 is determined by the transfer integral $t_\perp$ between adjacent chains.[10] In HTSC's the chains may be regarded as more of a quasi-one-dimensional nature with strong overlap ($t_\perp$) along at least the c direction. Therefore the T^2 behavior of ρ_{chain} would be in accordance with ee scattering.

At high temperature the chain resistivity ρ_{chain} approaches a temperature dependence $\rho\propto T^\lambda$ with $\lambda=\frac{4}{3}$ as shown in a log-log plot in Fig. 2. This temperature dependence extends from about 550 K to the highest measured temperature of 900 K. We also marked the Debye temperature $\Theta_D\approx 460$ K as deduced from specific-heat measurements.[11] The coincidence of the Debye temperature with the leveling off of ρ_{chain} at high temperatures seems to suggest a significance of phonons for the scattering mechanism along the chain. On the basis of a quadratic electron-phonon coupling theory for one-dimensional organic metals[12] a resistivity also proportional to T^2 has been predicted at low temperature. The strong electron-phonon coupling implies a strong pressure dependence of the resistivity. The experimental ratio[13] of the relative change of the resistivity ρ_b with the relative change of the lattice constant b, $d\ \ln\rho_b/d\ \ln b$, has been measured as 6.1 being lower than the values known for organic one-dimensional metals.[12] Further investigations will clarify the

situation of whether *ee*- or electron-phonon scattering or a combination of both is accurate to describe the charge dynamics inside the CuO chains.

Independent of the exact scattering mechanism for the resistivity along the CuO chain, 1:2:4 has given evidence of two different phases of free carriers. One phase are highly correlated carriers inside the CuO_2 plane with a scattering mechanism which is mainly determined by the dynamical magnetic susceptibility. For the CuO chains, we postulate another metallic ground state with itinerant carriers following $\rho \propto T^2$ at low T. The NQR measurements of the chain Cu(1) support the Fermi character of the carrier inside the chains as a Korringa-like law has been found. The Korringa ratio of 0.27 indicates a weak antiferromagnetic correlation of the itinerant carriers of the conduction channel along the chain.[14] In addition the spin-lattice relaxation time T_1 of Cu(1) has revealed only a minor change on cooling down from above to below T_c suggesting that the dynamics of the free carriers inside the CuO chain is not significantly modified by the phase transition to a superconductor.[15] Below T_c the structure of 1:2:4 might therefore consist of superconductor-metal-superconductor layers along the c direction with superconductivity along the c direction generated by the proximity effect. This is complimentary to the prevailing assumption of superconductor-insulator-superconductor junctions along the c direction in HTSC's.

Assuming a quasi-two-dimensional Fermi liquid for the CuO_2 planes with induced superconductivity along the c direction, Kresin, Morawitz, and Wolf[3] concluded the chain to be metallic. They also predicted two different gap values for the plane and the chain which, indeed, has been found for 1:2:4.[16]

A metallic ground state has also been suggested for the single CuO chain of fully oxygenated 1:2:3. A linear term in the thermal conductivity[17] as well as transport measurements along the b direction[18] have been attributed to free carriers inside the chains. Polarized far infrared reflectivity measurements also point to the significant contribution of the chain carriers to the conductivity.[19] The existence of two different kinds of charge carriers may be the cause that both, Fermi- and non-Fermi-liquid models, have partly been successful in explaining experiments.

In summary we have calculated the resistivity of the CuO chain of $YBa_2Cu_4O_8$ on assuming a model of shunted conduction channels (plane and chain) for the resistivity along the b direction. The resistivity of the chain ρ_{chain} follows a T^2 law for temperatures below 300 K and approaches a $T^{4/3}$ behavior at higher temperatures. The actuality of free carriers not belonging to the CuO_2 plane calls for careful interpretation of so-called ab-plane measurements in spectroscopic as well as thermodynamical experiments.

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