

Electron-lattice coupling and stripe formation in $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$

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The temperature dependence of the resistance $R(T)$ and the thermoelectric power $\alpha(T)$ under different hydrostatic pressures P are reported for polycrystalline $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$, $0.11 \leq x \leq 14$; they reveal a minimum in $R(T)$ and an abrupt change in the sign of $\alpha(T)$ at a transition from the low-temperature tetragonal (LTT) to the low-temperature orthorhombic phase. Superconductivity is suppressed at ambient pressure in the range $0.12 \leq x \leq 0.13$, where neutron-diffraction data have shown a static charge ordering into hole-rich and magnetic stripes, but pressure introduces n -type superconductivity into these compositions within the LTT phase with a $dT_0/dP \approx 1.0$ K/kbar. The $x=0.14$ sample is superconductive at ambient pressure in the LTT phase, and $dT_0/dP > 0$ changes to $dT_0/dP = 0$ at a $P_c \approx 10$ kbar. No anomaly in the transport properties is found at the magnetic ordering temperature $T_N \approx 30$ K in the LTT phase. These data, which show no support for stripe formation and superconductivity resulting from magnetic interactions, are found to be compatible with a model of strong coupling of charge carriers in coherent electronic states to fluctuations in the Cu-O bond lengths. Periodically alternating stripes of hole-rich and magnetic domains in the CuO_2 sheets are pinned, for $x \approx 1/8$, by the crystallographic distortion of the LTT phase; but the application of hydrostatic pressure, which decreases the magnitude of the LTT deformation, restores superconductivity apparently by depinning the stripes. [S0163-1829(97)09234-5]

INTRODUCTION

At high temperatures, the superconductive systems $L_{2-x}A_x\text{CuO}_4$, L =rare earth and A =alkaline earth, are tetragonal with CuO_2 planes alternating with $L_{2-x}A_x\text{O}_2$ rock-salt layers on traversing the c axis. This high-temperature tetragonal (HTT) phase remains stable to lowest temperatures at higher values of x ($x > 0.2$). For smaller values of x , the mismatch between the mean equilibrium L,A -O bond length and the equilibrium Cu-O bond length in the CuO_2 planes places the in-plane Cu-O bonds under a compressive stress. The bond length mismatch increases with decreasing temperature because of a smaller thermal expansion of the equilibrium Cu-O bond length; and below a transition temperature T_t , the compressive stress on the CuO_2 planes is relieved by a cooperative rotation of the CuO_6 octahedra around the $[110]$ axes, which lowers the symmetry from tetragonal to orthorhombic. In the low-temperature orthorhombic (LTO) phase, the 180° Cu-O-Cu bonds of the CuO_2 planes are buckled to $(180^\circ - \phi)$, transforming the planes to sheets.¹ The LTO-HTT transition temperature T_t decreases monotonically with increasing x .

In the system $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$, there is a second crystallographic transition below a $T_{t2} < T_t$ in a narrow compositional range $0.11 < x \leq 0.15$; in the low-temperature tetragonal (LTT) phase stabilized below T_{t2} , the CuO_6 octahedra rotate alternately about $[100]$ and $[010]$ axes of a CuO_2 sheet on traversing the c axis.² At compositions close to $x=1/8$ within the LTT phase field, superconductivity is suppressed; in $x=1/8$ compositions exhibiting similar behavior, static "stripes" parallel to $[100]$ or $[010]$ axes of the CuO_2 sheets have been observed to appear abruptly below T_{t2} by neutron diffraction.^{2,3} The existence of these stripes has also been demonstrated by EXAFS.^{4,5} Significantly, a high resolution

synchrotron x-ray diffraction study of a composition with $x=0.15$ has shown that superconductivity exists in the LTT phase,⁶ although with a reduced T_c , and static stripes were found only in samples where superconductivity is suppressed. However, inelastic neutron-scattering data are compatible with the presence of mobile stripes in a superconductive $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ composition with the LTO structure.⁷ These observations add strong support to heterogeneous electronic models of the copper-oxide superconductors that would segregate holes and spins into hole-rich and hole-poor domains. Moreover, in-plane thermal conductivity data provide striking evidence for a scattering of acoustic phonons by mobile "stripes," but not by the pinned stripes.⁸

Although the existence of mobile stripe domains in a magnetic matrix now appears firmly established for the normal state of the copper-oxide superconductors, the driving force for their formation remains controversial. In order to simplify the description of a complex system of interacting charges, spins and lattice vibrations, emphasis has been given to one feature or another. One approach would emphasize the electron-electron and magnetic interactions, as in a t - J model;⁹ another invokes the inherent lattice instability associated with the location of the Fermi energy ϵ_F in a van Hove singularity where the density $N(\epsilon_F)$ of one-particle states is exceptionally high.¹⁰ We,¹¹⁻¹⁴ on the other hand, have pointed out that a transition from localized (or strongly correlated) to itinerant electronic behavior may introduce a double-well potential for the equilibrium Cu-O bond length that would favor a segregation into hole-rich and magnetic domains. Moreover, where that segregation gives rise to an ordered alteration of the two types of domains, the heterogeneous state would represent a distinguishable thermodynamic phase.

Our thermoelectric power data indicated that formation of the distinguishable thermodynamic phase occurs by the con-

densation of a gas of nonadiabatic polarons containing several copper centers rather than by a van Hove instability. However, the data forced us to introduce local, dynamic pseudo-Jahn-Teller deformations of the oxidized copper centers; cooperativity among the local deformations was shown to stabilize polarons containing several copper centers and to introduce an elastic coupling between polarons that can compete with the Coulomb repulsion between them.¹⁵ Condensation of the polarons into extended domains introduces coherent electronic states having a dispersion $\epsilon(\mathbf{k})$ and a defined Fermi surface; these coherent states coexist with incoherent (localized) states in the lower Hubbard band (LHB) of the magnetic domains that lie well below ϵ_F . A gap at half-band in the coherent states makes the coherent charge carriers p type.

In this paper, we report the temperature dependence of the resistance $R(T)$ and of the thermoelectric power $\alpha(T)$ under different hydrostatic pressures for polycrystalline samples of $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ in the narrow compositional range $0.11 \leq x \leq 0.14$, and we argue that these data and similar measurements on the system $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ provide evidence for a $\partial N(\epsilon_F)/\partial\phi < 0$, or a $\partial n_{\text{eff}}/\partial\phi < 0$, where ϕ is a measure of the bending of the $(180^\circ - \phi)$ Cu-O-Cu bond angle and n_{eff} is the effective density of mobile charge carriers. On the other hand, the spin system appears to have little influence on the transport properties. These findings provide a strong indication that the electron-lattice, not the magnetic, interactions control the formation of the electronically heterogeneous thermodynamic phase found for the normal state of the copper-oxide superconductors.

EXPERIMENT

Samples of $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ were made from La_2O_3 , BaCO_3 , and CuO powders by conventional solid-state reaction. The samples were sintered at 1050°C followed by an anneal in oxygen atmosphere at 900°C . All samples were single phase to x-ray diffraction. Comparison of our data with the literature indicates that there is little, if any, deviation from oxygen stoichiometry.

Four-probe resistance $R(T)$ and thermoelectric-power $\alpha(T)$ measurements under high pressure were carried out in a self-clamped apparatus described elsewhere.¹⁶ The contribution to $\alpha(T)$ from the copper leads was subtracted out. The accuracy of the $\alpha(T)$ measurements is $\pm 0.3 \mu\text{V/K}$.

We use T_0 in place of the superconductive critical temperature T_c ; it is defined as the temperature below which the resistance becomes unobservable with a nanovolt meter. The pressures used to calculate dT_0/dP were measured at T_0 .

RESULTS

The evolution of the transport properties with hole doping x in $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$, $0.11 \leq x \leq 0.14$, can be separated into three compositional ranges: $x \leq 0.11$, $0.12 \leq x \leq 0.13$, and $x = 0.14$.

$x \leq 0.11$. Figure 1(a) shows the $R(T)$ and $\alpha(T)$ data for $x = 0.11$ under several applied pressures; the data are typical for compositions $x \leq 0.11$. The resistivity changes monotonically with temperature above T_c ; T_c increases with pressure with $dT_0/dP \approx 1.0 \text{ K/kbar}$. The origin of the change of slope

near 50 K in the ambient-pressure $R(T)$ curve is not identified. The $\alpha(T)$ curves are typical of an underdoped sample;¹² $\alpha(T)$ increases with temperature to a value that is temperature-independent, and the low-temperature enhancement peaking in the interval $100 < T_{\text{max}} \leq 150 \text{ K}$ in optimally doped samples is not apparent. Pressure increases not only T_c , but also $\alpha(T)$ of the normal state; see inset of Fig. 1(a).

$0.12 \leq x \leq 0.13$. Figures 1(b)–1(d) shows the $R(T)$ and $\alpha(T)$ data under several applied pressures for $x = 0.12$, 0.125 , and 0.13 . In this compositional range, superconductivity is suppressed at ambient pressure and a resistance minimum occurs at a $T_{\text{min}} \approx 70 \text{ K}$. Pressure reduces T_{min} , but it remains above 50 K under the highest pressures applied. As noted by others,^{17–20} pressure induces the appearance of superconductivity with a quite large dT_0/dP .

A remarkable drop in $\alpha(T)$ sets in on lowering the temperature through T_{min} , $\alpha(T)$ becoming negative at lower temperatures. A negative $\alpha(T)$ in the LTT phase has also been reported by others.^{21–24} Moreover, a low-temperature enhancement $\delta\alpha(T)$ with a $T_{\text{max}} \approx 150 \text{ K}$ emerges; it becomes more pronounced with increasing pressure as is evident, for example, in Fig. 1(d) for $x = 0.13$. Pressure also reduces the magnitude of the negative values of $\alpha(T)$; nevertheless, the superconductive state having $\alpha(T) = 0$, which is obtained at higher pressures, is approached on lowering the temperature from negative values of $\alpha(T)$. The superconductive state of the p -type superconductors is normally approached from positive values of $\alpha(T)$ as occurs for $x = 0.11$.

$x = 0.14$. Figure 1(e) shows the $R(T)$ and $\alpha(T)$ curves for $x = 0.14$ under several applied pressures. The data are similar to those obtained for $x = 0.13$, Fig. 1(d), except for the appearance of superconductivity at ambient pressure and a vanishing at higher pressure of dT_0/dP and $d\alpha(285 \text{ K})/dP$. The critical pressure (5 kbars) for a $d\alpha/dP = 0$ at 285 K is somewhat lower than the 10 kbars for $dT_0/dP = 0$.

DISCUSSION

Large single crystals of $\text{La}_{1.48}\text{Nd}_{0.40}\text{Sr}_{0.12}\text{CuO}_4$ appear to be more easily prepared than single crystals of $\text{La}_{1.88}\text{Ba}_{0.12}\text{CuO}_4$. Both compounds manifest the $x = 1/8$ suppression of superconductivity within a LTT phase field, and the phase diagrams of the two compounds are nearly identical; it is therefore appropriate to begin the discussion of our data with a review of the major results obtained by neutron-diffraction and resistivity measurements on single-crystal $\text{La}_{1.48}\text{Nd}_{0.40}\text{Sr}_{0.12}\text{CuO}_4$. Tranquada *et al.*³ found (a) a phase transition from LTT to LTO at a $T_{l2} \approx 70 \text{ K}$; (b) the abrupt appearance in the CuO_2 sheets of static stripes oriented parallel to $[100]$ or $[010]$ axes on lowering the temperature through T_{l2} ; (c) a long-range magnetic ordering within the hole-poor stripes below a $T_N \approx 50 \text{ K}$; (d) a discontinuity at a minimum in the resistivity $\rho_{ab}(T)$ of the a - b planes, i.e., CuO_2 sheets, at a $T_{\text{min}} = T_{l2} \approx 70 \text{ K}$; and (e) a smooth variation of $\rho(T)$ through T_N .

We find a $T_{\text{min}} \approx 70 \text{ K}$ in our $R(T)$ data also, which we take to mark the LTT-LTO transition at $T_{l2} < T_l$ in the range $0.12 \leq x \leq 0.14$ in $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$. There is no evidence for a LTT phase in the $x = 0.11$ sample; a T_{min} associated with the LTT-LTO transition disappears in the range $0.15 < x < 0.16$,

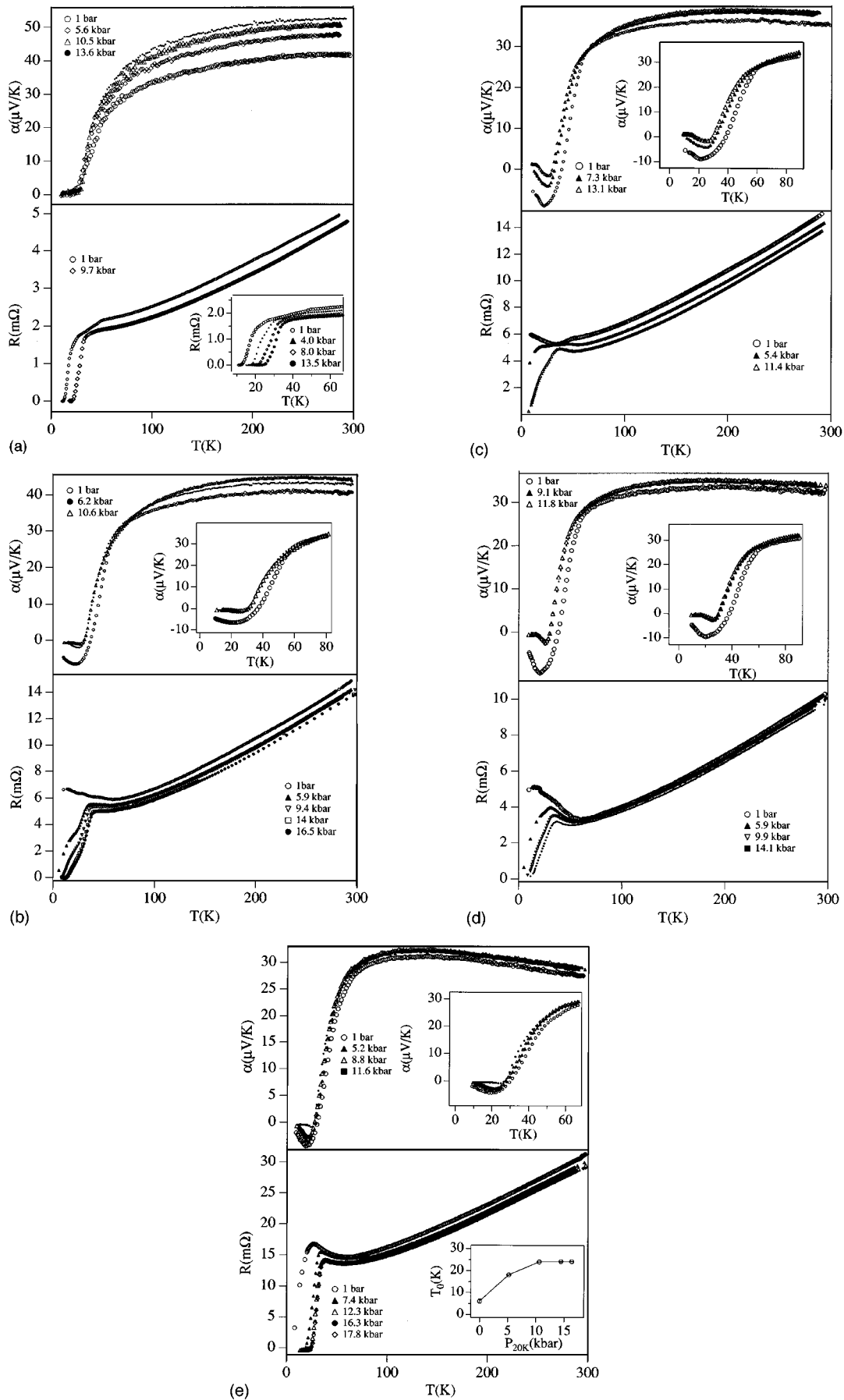


FIG. 1. Temperature dependence of the thermoelectric power $\alpha(T)$, and the resistance $R(T)$, under different hydrostatic pressures for polycrystalline samples of the system $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$: (a) $x=0.11$, (b) $x=0.12$, (c) $x=0.125$, (d) $x=0.13$, and (e) $x=0.14$.

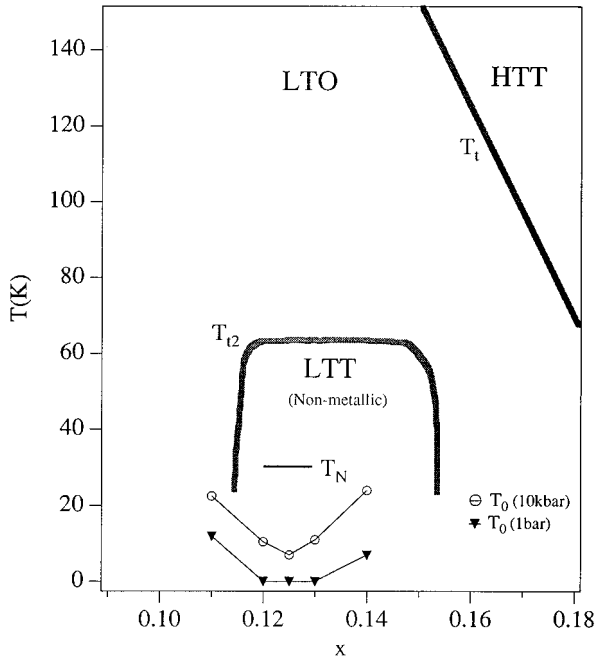


FIG. 2. Low-temperature phase diagram for the system $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$, $0 \leq x \leq 0.14$.

which gives us the tentative phase diagram shown in Fig. 2. NMR (Ref. 25) and μSR (Ref. 26) measurements have located a $T_N \approx 30$ K within the LTT phase field. The LTO-HTT transition temperature T_t is taken from neutron-diffraction data.²⁷

By analogy with $\text{La}_{1.48}\text{Nd}_{0.40}\text{Sr}_{0.12}\text{CuO}_4$, suppression of superconductivity in the range $0.12 \leq x \leq 0.13$ within the LTT phase is assumed to be associated with the formation of static stripes. We note that the stripes are oriented parallel to the [100] or [010] axes of the CuO_2 sheets whereas the rotations of the CuO_6 octahedra in the LTO phase are about [110] axes. In the HTT phase, there is no deformation to pin the stripes, so they remain mobile. In the LTO phase, the deformation axes cross the stripe axes at a 45° angle, so the deformation has a wrong symmetry for pinning the stripes. However, in the LTT phase the symmetry of the deformation is compatible with the pinning of stripes having widths commensurate with the lattice distortion. Commensuration can

occur only at a specific hole concentration, and the observation of static stripes at $x = 1/8$ within the LTT phase is the result of pinning by such a commensuration. The stripes are not pinned in the superconductive $x = 0.14$ sample.

In the CuO_2 sheets, phase segregation into large, nonadiabatic polarons in underdoped samples or stripe domains at higher hole concentrations would be accomplished by cooperative displacements of the oxygen atoms away from the magnetic Cu atom near neighbor toward the other nonmagnetic Cu atom at the boundary between phases, and these cooperative displacements may be either dynamic or static. At a critical composition, a competition between dynamic and pinned oxygen displacements could manifest itself in a large $^{16}\text{O}/^{18}\text{O}$ isotope effect, as has been observed²⁸ in the system $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ near $x = 1/8$. Moreover, mobile stripes would introduce dynamic oxygen displacements that could scatter strongly acoustic phonons transporting heat.

The parent compound La_2CuO_4 is a Mott-Hubbard anti-ferromagnetic semiconductor. Doping with an alkaline-earth atom A in the systems $\text{La}_{2-x}A_x\text{CuO}_4$ results in a large Fermi surface even in the underdoped cuprate;²⁹ it does not drop the Fermi energy ϵ_F into the lower Hubbard band, but transfers states from the incoherent Hubbard bands to the neighborhood of ϵ_F . We proposed a few years ago that these transferred states are associated with hole-rich, mobile domains that, for $x > 0.1$, condense into a thermodynamically distinguishable phase in the superconductive compositional range.^{12,13} The normal state of this new phase now appears to consist of fluctuating stripes of alternating hole-rich and hole-poor domains although the coherent states near ϵ_F exhibit a Fermi surface, as determined by ARPES, that is located close to the position predicted by band calculation. A positive thermoelectric power and Hall effect indicate that ϵ_F is located in a region of the dispersion curve that has a positive curvature as at the top of a band, and a mid-IR structure in UPS (Ref. 30) has provided evidence for a possible gap near ϵ_F in the middle of the band. We have discussed a possible origin of an energy gap at half-band¹³ as is illustrated schematically in Fig. 3(a). Angle-resolved photoemission spectroscopy (ARPES) has shown that in the region of ϵ_F , the dispersion curve is anomalously flat at the M point, which is in the direction of the Cu-O-Cu bond axes.³¹

Near $x = 1/8$ in $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$, a change in the sign of

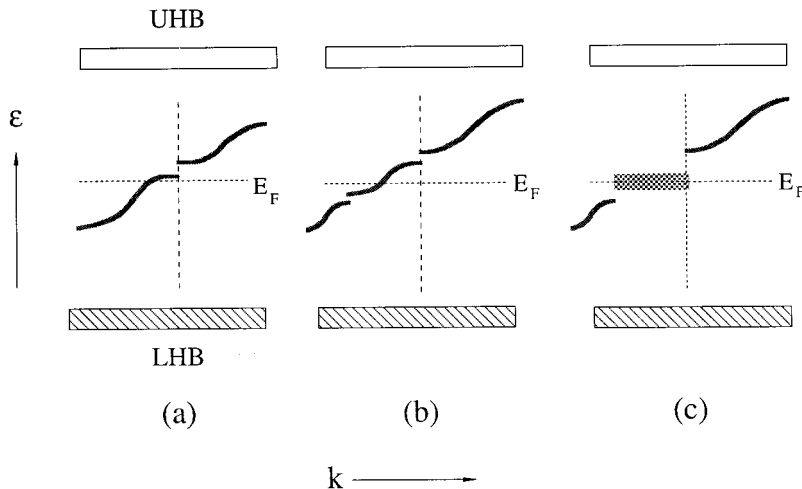


FIG. 3. Schematic $\epsilon(\mathbf{k})$ dispersion curves for $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$, $0.11 \leq x \leq 0.14$, in (a) the LTO and HTT phases and (b), (c) the LTT phase.

the thermoelectric power on cooling through the LTO-LTT transition temperature T_{12} is accompanied by a change in the resistivity $\rho(T)$ from a metallic to a semiconductive temperature dependence. A change in the sign of α signals a change in the sign of the curvature, averaged over all the Fermi surface, of the $\epsilon(\mathbf{k})$ dispersion curve at ϵ_F if a band model for the states near ϵ_F remains valid. Such a change would seem to require the opening of an energy gap below ϵ_F as illustrated in Fig. 3(b). Whether the gap at half-band remains in the LTT phase remains to be tested, but it should not be expected to vanish in the LTT phase as it is not related to the translational symmetry of the unit cell. From our model of the origin of the gap,¹³ we would expect the gap at half-band to increase with a pinning of the stripes that increases the bending ϕ of the Cu-O-Cu bonds from 180° .³² According to the model of Fig. 3(b), $|\alpha|$ should increase as ϵ_F approaches the lower band gap with increasing x , but we observe that $|\alpha|$ reaches a maximum at $x=1/8$. This latter observation suggests an alternative solution; the transition from the LTO to the LTT phase induces a separated band of polaronic states at ϵ_F that is located in a gap in the $\epsilon(\mathbf{k})$ curve as pictured in Fig. 3(c). Moreover, neutron diffraction data³² show that pinning of the stripes, which increases the bending ϕ of the Cu-O-Cu bond angle, narrows the bandwidth of the states near ϵ_F , and also traps out mobile charge carriers. At $x=1/8$, the Cu(III)/Cu ratio matches commensuration of the stripes, thereby minimizing the number of mobile charge carriers. This model is consistent not only with the observation of a nonmetallic temperature dependence of $\rho(T)$ below T_{12} , but also with a maximum $|\alpha|$ at $x=1/8$ since polaronic mobile charge carriers at ϵ_F would make the statistical contribution dominate the transport term in the thermoelectric power. Since the bending angle ϕ is a maximum for a commensurate pinning of the stripe domains at $x=1/8$, we conclude that the n_{eff} decreases as ϕ increases, i.e., $\partial n_{\text{eff}}/\partial\phi < 0$ or, for a band model with $n_{\text{eff}} \sim N(\epsilon_F)$, $\partial N(\epsilon_F)/\partial\phi < 0$. Moreover, a larger thermal expansion of the La-O and Ba-O equilibrium bond lengths relative to the Cu-O bond length makes the bond-length mismatch increase with decreasing temperature to give a $\partial\phi/\partial T < 0$.³³ Therefore the nonmetallic temperature dependence of the resistivity below T_{12} may reflect a $dn_{\text{eff}}/dT = (\partial n_{\text{eff}}/\partial\phi)(\partial\phi/\partial T) > 0$ rather than an activated mobility in the LTT phase.

We now consider the changes induced by pressure. In the LTT phase, a $dT_c/dP > 0$ is similar to that found in the LTO phase of the $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ system where pressure was found to stabilize the HTT phase relative to the LTO phase because $\partial\phi/\partial P < 0$.³⁴ The unusually high compressibility of the Cu-O bond in the superconductive compositions also applies to the $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ system to give a $\partial\phi/\partial P < 0$ (Ref. 20) in the compositions investigated in this study. It then follows that the observed $d|\alpha|/dP = (\partial|\alpha|/\partial n_{\text{eff}})(\partial n_{\text{eff}}/\partial\phi)(\partial\phi/\partial P) < 0$ requires a $\partial n_{\text{eff}}/\partial\phi < 0$ since $\partial|\alpha|/\partial n_{\text{eff}} < 0$. We can also demonstrate the relation $\partial n_{\text{eff}}/\partial\phi < 0$ from the observation that $dT_c/dP > 0$. From μSR data,³⁵ we have the relation $T_c \sim n_{\text{eff}}/m^*$, which gives $dT_c/dP \sim dn_{\text{eff}}/dP = (\partial n_{\text{eff}}/\partial\phi)(\partial\phi/\partial P) > 0$, and $\partial\phi/\partial P < 0$ then requires a $\partial n_{\text{eff}}/\partial\phi < 0$.

The pressure dependence of $|\alpha|$ shows a $\partial n_{\text{eff}}/\partial P > 0$. In an itinerant-electron model, the magnitude of $n_{\text{eff}} \sim N(\epsilon_F)$ depends on two factors, the flatness of $\epsilon(\mathbf{k})$ at ϵ_F and the total

density of itinerant-electron states. Since the width W_σ of the x^2-y^2 band of itinerant-electron states varies as $\cos\phi$ and we have a $\partial\phi/\partial P < 0$, W_σ must increase with pressure as the overlap integrals entering W_σ also increase with pressure. Therefore we conclude that the density n_{eff} of mobile charge carriers, whether polaronic or itinerant, increases with pressure in the LTT phase due to a transfer of spectral weight from trapped states to mobile-carrier states as ϕ decreases. In real space, the spectral-weight transfer would be associated with an increase with decreasing ϕ in the width of the hole-rich stripes once the stripes become depinned at a $\phi < \phi_c$. The data are thus consistent with the conclusion that superconductivity is found where the stripes are mobile.

We have shown elsewhere³⁶ that a $d[\delta\alpha(T)]/dP > 0$ in the LTO phase vanishes in the HTT phase as does dT_c/dP , which shows a $\partial[\delta\alpha(T)]/\partial\phi < 0$; therefore an increase in $N(\epsilon_F)$ also increases the enhancement term $\delta\alpha(T)$. The temperature at which $\delta\alpha(T)$ is a maximum falls in the range $100 < T < 150$ K, which is too high for acoustic phonons.³⁷ We conclude that $\delta\alpha(T)$ implies a strong coupling of the mobile charge carriers to the oxygen-atom displacements in the Cu-O-Cu bonds and a transfer of optical-mode lattice entropy by the charge carriers in the mobile hole-rich stripes.

Incommensuration of the stripe periodicity in the $x=0.14$ sample leads to a depinning of the stripes at ambient pressure; depinning reduces the bond bending to $\phi < \phi_c$ in the LTT phase and $N(\epsilon_F)$ becomes high enough to support superconductivity. We interpret a nearly pressure-independent $\alpha(285\text{ K})$ above 5 kbars to reflect a disappearance of the LTO fluctuations in the HTT phase³⁶ above 5 kbars at room temperature. On the other hand, a $dT_0/dP > 0$ vanishing above a $P_c \approx 10$ kbars within the LTT phase is interesting since an $\alpha < 0$ shows retention of the LTT phase to $P > P_c$, which indicates a $\partial\phi/\partial P < 0$ continues to be present for $P > P_c$. It would appear that a depinning of the stripes that releases all the trapped carriers is not complete for $P < P_c$ and that once the release of trapped carriers is complete at $P > P_c$ there is little dependence of T_0 on ϕ in the LTT phase.

For $x=0.16$, the LTO phase is retained to lowest temperatures and, on cooling through T_c , $\alpha(T)$ drops to zero from the positive side. Moreover, a $dT_c/dP > 0$ to 17 kbars shows, unlike the LTT phase, a marked $dT_c/d\phi < 0$ as in the LTO phase of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$.³⁸ This observation suggests there is an important transfer of spectral weight from the Hubbard bands to the coherent band with decreasing ϕ in the LTO phase that does not occur in the LTT phase.

Finally, the band model successfully predicts the locus of the Fermi surface obtained by ARPES whereas real-space experiments have now shown the presence of dynamic hole-rich and hole-poor stripes in most of the high- T_c cuprate systems.²⁻⁵ With a photoemission resolution of $\Delta E \approx 20$ meV, ARPES may not be able to resolve the band structure changes induced by stripe formation if the stripes are mobile with a short residence time Δt on a given atom.

SUMMARY AND CONCLUSIONS

In summary, we have found the following.

- (1) Both $R(T)$ and $\alpha(T)$ show no anomaly at a magnetic-

ordering temperature or, as we have shown elsewhere,³⁹ at the opening of a spin gap; however, they both change dramatically at the structural LTT-LTO transition temperature T_{12} and they both vary sensitively with the bending ϕ of the $(180^\circ - \phi)$ Cu-O-Cu bonds.

(2) The normal state of the superconductive compositions is a distinguishable thermodynamic state consisting of a periodic array of alternating hole-rich and magnetic domains (stripes) that are mobile, and at a ratio Cu(III)/Cu=1/8, the period of this charge-density wave (CDW) is commensurate with the lattice periodicity of a CuO_2 sheet. However, pinning of the CDW to give static stripes observable by diffraction experiments only occurs in the LTT phases.

(3) Formation of the stripes does not introduce an energy gap at ϵ_F , which would suppress superconductivity, either where the stripes are mobile or become pinned in the LTT phase; but a gap at midband in the (x^2-y^2) band of coherent states makes the charge carriers p -type in the HTT and LTO phases, the opening of an additional gap below ϵ_F by the structural change makes the charge carriers n -type in the LTT phase.

(4) In both the LTO and LTT phases, hydrostatic pressure reduces the bending ϕ of the $(180^\circ - \phi)$ Cu-O-Cu bond angle: $\partial\phi/\partial P < 0$, which is indicative of an exceptionally compressible mean equilibrium Cu-O bond length, i.e., of a double-well bond potential.

(5) A $\partial T_c/\partial\phi < 0$ implies a $\partial n_{\text{eff}}/\partial\phi < 0$, where $n_{\text{eff}} \sim N(\epsilon_F)$ is the effective density of coherent electronic states at ϵ_F , i.e., $\partial N(\epsilon_F)/\partial\phi < 0$.

(6) In the LTO phase, a $\partial W_\sigma/\partial\phi < 0$ for the width W_σ of the x^2-y^2 band of coherent states promotes a transfer of spectral weight from incoherent to coherent states with decreasing bending ϕ of the $(180^\circ - \phi)$ Cu-O-Cu bond angle; this spectral-weight transfer appears to accompany a mean flattening of the $\epsilon(\mathbf{k})$ dispersion curves at ϵ_F . In the LTT

phase, the flat portion of the dispersion curve appears to transform to a set of polaronic states within a gap in the dispersion curve for the coherent states, and the number of mobile polaronic states increases with decreasing ϕ and depinning of the stripes.

(7) The bending ϕ of the $(180^\circ - \phi)$ Cu-O-Cu bond angles is a maximum and $N(\epsilon_F)$ is therefore a minimum where the stripes are pinned and superconductivity is suppressed; reduction of ϕ to a $\phi < \phi_c$ by hydrostatic pressure depins the stripes and introduces superconductivity.

(8) A $\partial[\delta\alpha(T)]/\partial P > 0$ shows that the enhancement $\delta\alpha(T)$ of the thermoelectric power also increases with $N(\epsilon_F)$; a maximum in $\delta\alpha(T)$ in the temperature range $100 < T < 150$ K suggests that the mobile charge carriers transport optical-mode, not acoustic-mode, lattice entropy, which would be consistent with a strong coupling of the charge carriers to Cu-O bond-length fluctuations.

In conclusion, there is little evidence that magnetic or electron-electron interactions alone or the location of a Fermi energy in a van Hove singularity is responsible for the peculiar transport properties of the normal state of the copper-oxide superconductors. On the other hand, there is overwhelming evidence that strong electron coupling to fluctuations of the Cu-O bond lengths is occurring; these fluctuations would be the result of both a double-well potential for the Cu-O bond at a crossover from localized to itinerant electronic behavior and local, pseudo Jahn-Teller deformations. A recent study⁴⁰ of the insulator-metal transition in the system $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ occurring in a pulsed field of 61 T is completely consistent with this conclusion.

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