

Buckling of the CuO_2 Planes and the Electronic Properties of Doped La_2CuO_4 Superconductors

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The electronic properties of rare earth (RE) doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO) depend sensitively on the tilt displacements of the CuO_6 octahedra. In particular, in the low temperature tetragonal (LTT) phase with increasing tilt angle Φ a crossover from a metallic, superconducting to a metallic, non-superconducting phase with probably (local) antiferromagnetic (AF) order is observed. We discuss the influence of the tilt displacements on the electronic properties in the three structural low temperature phases of RE-doped LSCO.

The structural phase transition from the orthorhombic (LTO) to the tetragonal low temperature phase in RE doped LSCO has a strong influence on the electronic properties and can destroy superconductivity in a certain range of composition [1]. We discuss in this paper the relevance of the structural changes induced by doping with RE for the electronic properties of LSCO.

From a detailed analysis of the structural, transport and superconducting properties we have recently shown that it is not the hole concentration x alone, which determines the occurrence of electronic anomalies in the LTT phase [2]. Straightforward evidence for this is that the occurrence of superconductivity in the LTT-phase at fixed hole concentration x can be tuned via additional doping with Nd, since it is known that Nd-doping affects the structure only. From our experiments on a large number of samples with various Nd- and Sr-concentrations we find the two regions in the LTT phase shown in fig.1: In region I ($\Phi > \Phi_c$) strong transport anomalies occur and superconductivity is absent; in region II ($\Phi < \Phi_c$) bulk superconductivity is found and transport anomalies are absent. The line separating the two regions is a line of constant tilt angle of the CuO_6 octahedra and thus defines a critical tilt angle Φ_c .

The non-superconducting LTT-phase has electronic properties significantly different from those of the superconducting LTT and of the LTO phase. This is apparent from the behavior of the transport properties: The resistivity increases

at low temperatures; interestingly, the thermal conductivity increases also. The thermopower show a complicated behavior, strongly influenced by the hole concentration as we will discuss below. Moreover, (local) AF order has been observed by Mößbauer- and μSR -experiments with $T_N \approx 31\text{K}$ [3].

It is well known that the tilt displacements or equivalently the buckling pattern of the CuO_2 planes are coupled to the magnetic properties: In the undoped AF insulator La_2CuO_4 the tilt leads to a canting of the Cu spins out of the CuO_2 planes and results in weak ferromagnetism. This can be attributed to the spin-orbit coupling induced antisymmetric Dzyaloshinskii-Moriya (DM) interaction between the Cu spins.

Recently, Bonesteel et al. have suggested that in Sr-doped La_2CuO_4 the motion of the charge carriers is coupled to the tilt displacements via spin-orbit scattering [5]. Including this coupling into the t-J model they find a first order $T=0$ phase transition with increasing tilt angle from a spiral magnetic pattern to a commensurate AF state at finite doping concentrations. It is very appealing to relate this transition to the disappearance of superconductivity at the critical buckling found in our experiments, in particular in view of the (local) AF order observed in the non-superconducting LTT-phase. However, while the mere existence of Φ_c seems to support the results from this model, we know from the neutron diffraction data that the *magnitude* of the tilt angle does not change at T_{LT} . It is only the tilt *axis*

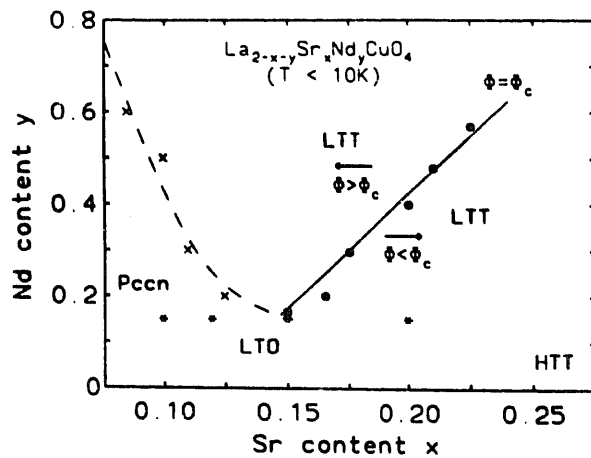


Figure 1. Schematic low temperature ($T < 10K$) phase diagram. The phase range of the high temperature tetragonal (HTT) phase was extrapolated from $T_{HT}(x, y)$. The dashed line marks the phase boundary between Pccn and LTT found for $y > 0.15$ and low x . The full line separating region I and II in the LTT phase is a line of constant tilt angle.

that changes. To capture this is beyond the single band model by Bonesteel et al., in which the magnitude of Φ is the only parameter to describe the influence of the tilt.

From our experiments we find that the influence of the tilt angle on the electronic properties is different in the three low temperature structural phases possible in LSCO, in which the tilt axis is different: It is very strong in the LTT-phase, as described above, weaker in the Pccn-phase and small in the LTO-phase.

Evidence for a small influence of the tilt in the LTO phase comes from the pressure dependence of T_c and the transition temperature T_{HT} for the structural transition between the high temperature tetragonal (HTT) and the LTO phase and from the dependence of T_c and T_{HT} on doping with Pr. One finds $(dT_c/dp)/(dT_{HT}/dp) \simeq (dT_c/dy)/(dT_{HT}/dy)$, where y denotes the Pr-concentration [6]. Moreover, also the thermal ex-

pansion anomalies of LSCO at T_c give evidence for a coupling of T_c to the tilt angle [7].

In the Pccn phase the tilt axis is in between those of the LTT and the LTO phase. Accordingly the influence of the tilt on the electronic properties is intermediate between that in the LTO and the LTT phase. Our experiments suggest that the component of tilt along the LTT direction determines the suppression of superconductivity.

We finally comment on the influence of the hole concentration. We do find a significant, in particular, non-monotonous influence of x on the electronic properties in the *non-superconducting* LTT phase. Evidence for this comes from the thermopower, which shows a pronounced sign change near a hole concentration of $x \approx 1/8$. This can be understood as a result of a splitted density of states peak as predicted on the basis of bandstructure calculations for the LTT-phase [8]. However, we emphasize that these calculations also predict an unsplit density of states peak in the LTO phase; yet, no anomalies of the thermopower as a function of doping are found. It thus seems that if bandstructure results are applicable only for the properties of the non-superconducting LTT-phase.

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REFERENCES

1. B. Büchner et al., *Physica C* **185-189**, 903 (1991); M.K. Crawford et al., *Phys. Rev. B* **44**, 7749 (1991)
2. B. Büchner et al., *Europhys. Lett.* **21**, 953 (1993); and submitted to *Phys. Rev. Lett.*
3. M. Breuer et al., *Z. Phys. B* **92**, 331 (1993)
4. D. Coffey et al., *Phys. Rev. B* **44**, 10112 (1991)
5. N. Bonesteel et al. *Phys. Rev. Lett.* **68**, 2684 (1992)
6. N. Yamada and M. Ido, *Physica C* **203**, 240 (1992); W. Schäfer et al., *Phys. Rev. B* **49**, 9248 (1994);
7. M. Braden et al., *Phys. Rev. B* **47**, 12288 (1993)
8. W.E. Pickett et al., *Phys. Rev. Lett.* **67** 228 (1991)