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## Band structure and electron-phonon coupling in the $\text{La}_{1-x}\text{Sr}_x\text{CuO}_4$ superconductors

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*In honor of Martin Peter's 60th birthday.*

**Abstract.** Self consistent LMTO band results for  $\text{La}_2\text{CuO}_4$ ,  $\text{LaSrCuO}_4$  and  $\text{Ba}_2\text{CuO}_4$  are used for calculations of the electron-phonon coupling. A relatively large variation of the charge transfer is found as the atomic distance between Cu and O on the  $z$ -axis is changing. This leads to enhanced electron-phonon coupling in  $\text{LaSrCuO}_4$ . The standard rigid-muffin-tin-approximation RMTA value of  $\lambda$  is smaller in  $\text{LaSrCuO}_4$  than in  $\text{La}_2\text{CuO}_4$  despite a larger density-of-states at the Fermi energy.

Theoretical studies of electron-phonon coupling  $\lambda$  and superconductivity on the basis of electronic structure calculations have been able to describe superconducting properties of many materials [1–3]. However, the recent discoveries of superconductivity in the range of 40–90 K in oxides [4, 5] have been a surprise. Electron-phonon coupling may be the mechanism for the high  $T_c$ 's in some of these materials while not in others [6, 7]. Various other models, in which sometimes the existence of a well defined bandstructure is questioned, have been proposed [8] and are being tested. In contrast to the newly proposed models, are calculations of electron-phonon coupling an established technique and it is possible to calculate most of the important parameters from first principles. In this paper we apply our methods to the  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  system (which is the less complicated of the two oxide structures) in order to study the bandstructure and its implication on  $\lambda$  and superconductivity.

The Linear-Muffin-Tin-Orbital band method is used to calculate the electronic structures self-consistently [2, 3]. The structure contains two empty spheres in addition to the atomic spheres, totally 9 sites per body centered tetragonal unit cell. The structural data are taken from Decroux et al. [9]. The resulting bandstructure for  $\text{La}_2\text{CuO}_4$  resembles those of Mattheiss [10], Yu et al. [11] and Temmerman et al. [12]. In particular the density-of-states Fig. 1a in ref. [12] resulting from a LMTO calculation is similar to ours. For  $\text{LaSrCuO}_4$  and  $\text{Ba}_2\text{CuO}_4$  we use the same structural data as for  $\text{La}_2\text{CuO}_4$ . The fewer number of valence electrons in Ba and Sr compared to La, introduces large changes in the DOS near  $E_F$ . However a rigid band picture is insufficient to describe the

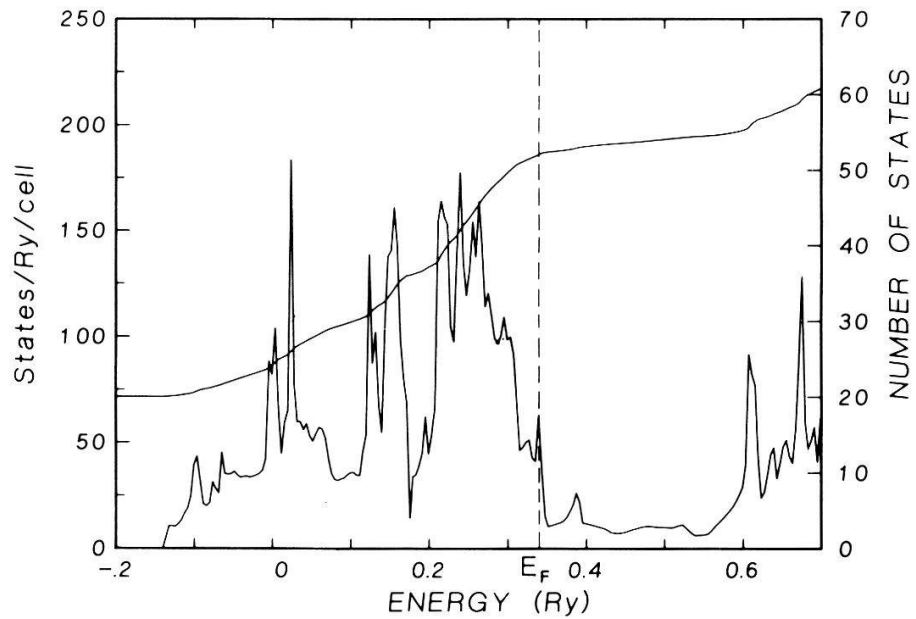


Figure 1  
Total density of states and number of valence states per unit cell calculated for LaSrCuO<sub>4</sub>.

changes. The anisotropy of the Fermi surface described as  $(V_x^2 + V_y^2)/2V_z^2$  where  $V_i$  is the bandvelocity in direction  $i$ , is about 10 for La<sub>2</sub>CuO<sub>4</sub> and Ba<sub>2</sub>CuO<sub>4</sub> and about 5 for LaBaCuO<sub>4</sub>, with  $\langle V_F \rangle$  2.3, 1.6 and  $1.1 \cdot 10^5$  m/s respectively. The ( $q = 0$ ) Stoner enhancement calculated for the unit cell as a whole is ranging between 1.3–2 for the three compositions. Strong Fermi surface nesting [10] may lead to spin-fluctuations which in supercell bandcalculations would show up as large  $q \neq 0$  Stoner enhancements.

The electron phonon coupling  $\lambda$  can be written  $NI^2/K$  where  $I$  is matrix element of the deformation potential  $\sum_{kk'} \langle \psi_k | dV/dr | \psi_{k'} \rangle$ . The density-of-states at  $E_F$  is  $N$  and  $K$  is the second derivative of the total energy with respect to the lattice deformations  $\Delta \bar{R}$  which are involved in the phonon displacements. The average of  $K$  is often written  $M\langle \omega^2 \rangle$  where  $\omega$  is a phonon frequency and  $M$  the atomic mass. In the rigid muffin-tin approximation (RMTA) one evaluates  $I^2$  through a rigid displacement of the  $MT$  potential, so that

$$\frac{dV}{dR} \cong \Delta \hat{R} \cdot \frac{dV(r)}{d\bar{r}}.$$

The resulting dipole operator couples  $l$  and  $l' = l \pm 1$  states. The effects of screening (or charge fluctuations) are lost through the assumption of rigid muffin-tins, and by doing 'frozen phonon' calculations one is able to improve the calculation of the matrix element. The potential after a deformation  $\Delta \bar{R}$ ,  $V(r + \Delta \bar{R})$  is in our case a  $MT$  potential with origin in a new coordinate system  $\bar{r}' = r + \Delta \bar{R}$ . The delocalized part of this potential can be described around the old coordinate system  $r$  as approximately  $V(r) + \Delta \bar{R} \cdot dV(r)/d\bar{r}$ . The change in potential,  $V(r + \Delta \bar{R}) - V_0(\bar{r})$ , where  $V_0(\bar{r})$  is the potential for the undeformed

lattice, can be written  $(V(r) - V_0(r)) + \Delta\vec{R} \cdot dV/d\vec{r}$ . Finally

$$\frac{\Delta V}{\Delta R} \cong \frac{V(r) - V_0(r)}{\Delta R} + \Delta\hat{R} \cdot \frac{dV}{d\vec{r}}.$$

In the RMTA  $V(r) = V_0(r)$  and only the second term remains. The first, monopole term may be of importance if there is a charge fluctuation associated with a particular phonon. Usually its contribution is negligible, whereas the main contribution comes from the second term. Here we calculate the second term using the RMTA, (the LMTO results use spherically symmetric potentials) although screening effects, if they are present, probably modify the dipole term as well. In these first calculations we include only the  $l=0$  part of the screening effects. The monopole term is calculated using  $V_0(r)$  and  $V(r)$  for the undeformed and deformed lattices, and as will be shown, the charge fluctuation induced by a particular phonon makes this term important.

The calculation of  $K$  requires precise calculations of differences of total energies and here non-spherical potential contributions are essential. Since our calculations are based on spherical muffin tin potentials it is safer to use experimental estimations of  $K$  rather than calculated values. From Raman measurements [13] on  $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$  one has obtained force constants ( $K$ ) for the  $\text{CuO}_\text{I}$  and  $\text{CuO}_\text{II}$  pairs of 5.3 and 1.3 eV/Å<sup>2</sup> respectively. (Here I refers to the oxygen atoms in the  $x$ - $y$  plane and II refers to an oxygen on the chain along the  $z$ -axis.) Inelastic neutron scattering measurements [14] on the same compound gives breathing modes involving I and II CuO pairs between 50 and 90 meV, while rotational and other modes involving oxygen is at lower energy about 30 meV. The phonon calculations of Weber [6], give a similar phonon spectrum.

In Table I we show the density of state values at  $E_F$  calculated for  $\text{La}_2\text{CuO}_4$ ,

Table I

	La <sub>2</sub>	Cu	O <sub>2</sub> (I)	O <sub>2</sub> (II)	
<i>s</i>	0.0	0.8	0.6	0.0	
<i>p</i>	0.0	0.2	4.2	1.2	
<i>d</i>	2.9	11	1.0	0.2	
<i>f</i>	0.1	0.0	0.4	0.0	
	La	Sr	Cu	O <sub>2</sub> (I)	O <sub>2</sub> (II)
<i>s</i>	0.1	0.3	0.4	0.1	0.1
<i>p</i>	0.4	0.2	0.2	6.1	20
<i>d</i>	1.6	0.8	14	0.3	0.1
<i>f</i>	0.5	0.4	0.0	0.2	0.0
	Ba <sub>2</sub>	Cu	O <sub>2</sub> (I)	O <sub>2</sub> (II)	
<i>s</i>	0.2	0.1	0.2	0.0	
<i>p</i>	1.1	0.2	4.8	25	
<i>d</i>	0.9	5.2	0.4	0.0	
<i>f</i>	0.6	0.0	0.1	0.0	

Partial density states per unit cell and Rydberg for the three compounds.

Table II

	$N(E_F)$ ( $\text{Ry} \cdot \text{cell}$ ) <sup>-1</sup>	$\lambda_{\text{RMTA}}$	$\lambda(\text{I})$	$\lambda(\text{II})$	$\lambda_{\text{TOT}}$	$T_c$ K	$\gamma$ mJ/(K <sup>2</sup> g-at)
La <sub>2</sub> CuO <sub>4</sub>	23	0.54	<0.01	0.10	0.6	7	0.7
LaSrCuO <sub>4</sub>	46	0.39	0.02	1.0	0.9	20	2.1

Calculated total DOS at  $E_F$ , the RMTA calculation of  $\lambda$ , the  $\Delta l = 0$  values for  $\lambda$  calculated for the two different CuO modes I and II, superconducting  $T_c$  using the total  $\lambda$  in the McMillan formula and electronic specific heat. In the calculation of  $\lambda$ , the phonon denominator is taken as an average over all CuO<sub>4</sub> modes (the contribution from La and Sr is negligible). Thus for  $M$  being the average atomic mass and for  $\hbar\omega$  being an average of 30 meV (obtained from different experiments in Refs. [13–14]) one estimates  $M\omega^2 = 5.4 \text{ eV}/\text{\AA}^2$ , and  $\lambda = \sum_{\text{atoms}} \eta_i / M\omega^2$ .  $\lambda_{\text{TOT}}$  is  $\lambda_{\text{RMTA}} + (\lambda(\text{I}) + \lambda(\text{II}))/2$ . In the calculation of  $T_c$  is  $\mu^* = 0.13$  and  $\theta_D = 475 \text{ K}$  [13]. It turns out that  $\eta_{\text{II}}$  is considerably larger than  $\eta_{\text{I}}$  so using softer  $\hbar\omega$ , for the O(II) mode instead of the averaged one, would make  $\lambda(\text{II})$  larger.

Ba<sub>2</sub>CuO<sub>4</sub> and LaSrCuO<sub>4</sub>. As is shown in Fig. 1  $E_F$  is just on a shoulder of a higher DOS region involving Cu- $d$  and O(II)- $p$  states in LaSrCuO<sub>4</sub>. A notable difference is that the degree of band admixture is smaller in the LaSrCuO<sub>4</sub> compound so that the standard RMTA value of  $\lambda$  is lower (see Table II) than in La<sub>2</sub>CuO<sub>4</sub> despite the higher DOS.

Two ‘frozen phonons’ are treated; one involves a displacement of the O(I) atoms in the  $xy$ -plane relative to the Cu atom, the other a ‘breathing’ displacement of the O(II) atoms on the  $z$ -axis relative to the Cu atom in between. With these displacements it is possible to study the effects of phonons from O(I) and (II) atoms and still work with the seven atom unit cell. The selfconsistent results calculated for the  $xy$ -plane phonon do not differ so much from the results calculated for the undistorted structure. In LaSrCuO<sub>4</sub> the Cu–O(I) charge exchange amounts to about  $0.07 \text{ e}^-/\text{a.u.}$ . The effects of the displacements of the O(II) atoms are larger: In the same compound the change of Cu charge is about  $0.39 \text{ e}^-/\text{a.u.}$  and in La<sub>2</sub>CuO<sub>4</sub> it is about  $0.14 \text{ e}^-/\text{a.u.}$ . In O(I) the charge changes about  $0.07 \text{ e}^-/\text{a.u.}$  (the inequivalent O(I) are averaged over in LaSrCuO<sub>4</sub>) and  $0.03 \text{ e}^-/\text{a.u.}$  for the two compounds respectively. The charge transfer on the O(I) atom is comparable to the one on O(II) although it is not displaced. These charge transfers are accompanied by large deformation potentials which can give large contributions to the  $\Delta l = 0$  electron phonon coupling if the DOS at  $E_F$  is large. In La<sub>2</sub>CuO<sub>4</sub> this is not the case and as is seen in Table II,  $\lambda(\text{I})$  and  $\lambda(\text{II})$  are small. But in LaSrCuO<sub>4</sub> it is seen that  $\lambda(\text{II})$  is very large compared to the RMTA contribution. The combined  $\lambda$  gives together with other parameters obtained from experiment a rather high  $T_c$  using the McMillan formula.

The results give an indication that electron phonon coupling assisted by charge fluctuations can be large for O(II) modes in the La<sub>2– $x$</sub> Sr <sub>$x$</sub> CuO<sub>4</sub> system. But refined calculations would also include enhancement due to charge fluctuations of the  $\Delta l = 1$  contribution to  $\lambda$ , which normally is the dominant contribution. This could further increase  $\lambda$ . But on the other hand, not only O(II) phonons should be included, which presumably makes the average  $\lambda$  lower.



The stability of the structure has not been considered here; soft phonons and high DOS may lead to new structures. Our large  $\lambda$  for  $\text{LaSrCuO}_4$  is conceivable with the high  $T_c$  in  $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$  is regions of Sr-rich  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  are superconducting and stabilized by regions of low DOS  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  which are poor of Sr. Further scrutiny of our results leads us to the 90 K superconductivity in the  $\text{YBaCuO}$  system and to the question if a similar mechanism may enhance  $\lambda$  for this system. Here, a weak isotope effect [16] is observed but calculations [7] suggest other mechanisms than electron-phonon coupling. Band calculations give large Cu(2), O(4) and O(I) DOS at  $E_F$  already at stoichiometric composition for  $\text{YBa}_2\text{Cu}_3\text{O}_7$  [16]. It appears that the DOS per O-site is larger than for our O(II) site in  $\text{LaSrCuO}_4$ . It might than be worthwhile to do calculations of the  $\Delta I = 0$  deformation potential also for this system, in particular by considering phonon modes involving O-sites on chain positions. In this respect it is interesting to find experimental evidence for a well defined Fermi surface [17], showing that on-site correlation is not too large, but that band theory should be able to describe its physical properties.

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