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Calculations of the Superconducting Properties of Cu-O Based Perovskite-Like Structures

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We have used the results of first principles local density band structure calculations to calculate the McMillan-Hopfield parameter η in a series of ordered cubic perovskite and layered perovskite structures of the form $M_xN_yCuO_z$, where M and N are La, Ba, and Cs. We find relatively low values of η compared to those of transition metal superconductors, but within a range of soft oxygen phonon modes the resulting electron-phonon coupling strength λ is large ($\lambda \sim 2.5$). This strength appears to be sufficient to explain the high transition temperatures T_c=30-40 K in these materials within the usual electron-phonon mechanism.

1. INTRODUCTION

The recent remarkable discoveries [1-4] of superconducting transition temperatures T_c in the range of 40-100 K in perovskite-like compounds, has raised the question as to whether the traditional electron-phonon mechanism is valid in these systems. We investigate this question using a method which has been highly successful in evaluating the superconducting properties of the previously known superconductors.

2. CALCULATIONS AND DISCUSSION

We have performed band structure calculations [5] for the system $La_{2-x}Ba_xCuO_{4-y}$ with x=0,1 and y=0. This alloy is a high temperature superconductor for small values of x and y, with a maximum T_c=40 K at x=0.15. We have used the results of the band calculations and the theory of Gaspari and Gyorffy [6] to calculate the McMillan-Hopfield parameter $\eta = N(E_F)\langle I^2\rangle$. The values of η together with the average electron-ion matrix elements $\langle I^2\rangle$ are given in Table I for each component of the layered compounds La_2CuO_4 and $LaBaCuO_4$ and for the x=0.14 material in the rigid band approximation. For comparison we have also performed similar calculations for the cubic perovskites $LaCuO_3$, $BaCuO_3$ and $CsCuO_3$ and the results are included in Table I. From Table I we note that $N(E_F)$ is significantly larger for the Ba than for the La compounds. However, in the Ba compounds the matrix elements $\langle I^2\rangle$ decrease moderately for the Cu site and substantially for the O sites.

As a result η, which is the product of $N(E_F)$ and $\langle I^2\rangle$, doesn't increase proportionally to $N(E_F)$. In fact η_O decreases from La_2CuO_4 to $LaBaCuO_4$ in spite of the factor of three increase in $N(E_F)$. An interesting point is that the values of η_{Cu} and $\eta_{O_{tot}}$ are fairly close between La_2CuO_4 and $LaCuO_3$ which suggests that the cubic-perovskite structure, if stable, might also provide high temperature superconductors.

If we consider the per atom value of both $N(E_F)$ and η in these materials it becomes clear that they both are significantly smaller than those of previously referred to as high temperature superconductors (A15 compounds, NbN, etc.). On the other hand an analogy can be drawn with PdH which has $N(E_F)$=0.48 states/eV, $\eta_{Pd}=0.86\frac{eV}{\text{Å}^2}$, $\eta_H=0.39\frac{eV}{\text{Å}^2}$ and $T_c \approx 10$ K. In PdH soft phonon modes associated with hydrogen vibrations have been shown to be responsible for the electron-phonon coupling [7].

In an attempt to raise the value of η in this class of materials we performed the same calculation for $CsCuO_3$. This calculation brings E_F into a high DOS region ($N(E_F)$=3.48 states/eV/spin) but due to a decrease in $\langle I^2\rangle$ the values of η, with the exception of η_{Cs}, remain close to those of the other compounds.

In this spirit we calculate the electron-phonon coupling λ as follows. We first write λ as a sum of contributions for the different atomic sites, i.e.

$$\lambda = \left(\frac{\eta_{La}}{M_{La}} + \frac{\eta_{Cu}}{M_{Cu}} + \frac{\eta_O}{M_O} \right) \frac{1}{\langle \omega^2 \rangle} \qquad (1)$$

where $\langle \omega^2 \rangle$ is an rms vibrational frequency. Because we find that $\eta_{La} \approx 0$ and because $M_{Cu} \gg M_O$ we can write,

$$\lambda = \frac{\eta_{Cu}}{M_{Cu}\omega_{Cu}^2} + \frac{\eta_O}{M_O \omega_O^2} . \qquad (2)$$

The average phonon frequencies ω_{Cu} and ω_O may be obtainable from Born-von Karman fits to neutron scattering measurements. However, since such analysis is not available at present we have made the simplifying assumption that

$$M_{Cu}\omega_{Cu}^2 = M_O \omega_O^2 \qquad (3),$$

which follows if Cu-O modes dominate the coupling to Fermi surface electrons. Treating ω_O as a variable parameter, we have calculated λ as a function of ω_O. Subsequently we calculate T_c using the Allen-Dynes equation [8]:

$$T_c = f_1 f_2 \frac{\omega_{log}}{1.2} \exp_2 \left[- \frac{1.04(1+\lambda)}{\lambda - \mu^* - 0.62\,\lambda\mu^*} \right] \qquad (4)$$

where μ^*=0.1 is the Coulomb pseudopotential the inclusion of the prefactors f_1 and f_2 are important for large values of λ as discussed by Allen and Dynes.

Our results for both λ and T_c as a function of ω_O are shown in Fig. 1 for x=0.0 and for x=0.14 based on a rigid band model evaluation (justified elsewhere) of $N(E_F)$ and η.

Figure 1 shows that for values ω_O close to 200 K λ is about 2.6 and T_c is about 35 K. This result indicates that as long as the average phonon frequency is in the above frequency range at least the 40 K superconductors can be understood within the conventional electron-phonon mechanism.

3. ACKNOWLEDGMENTS

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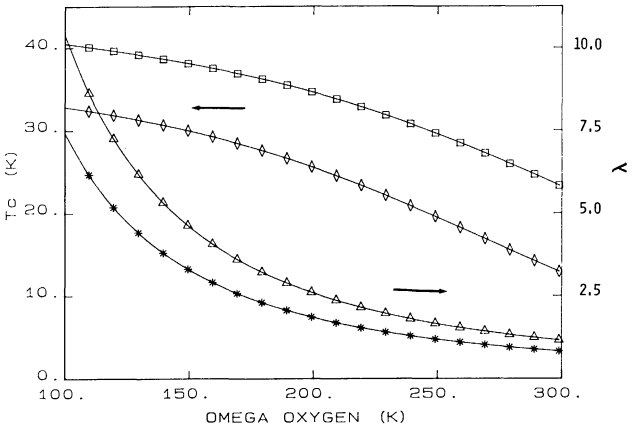

Figure 1. Calculated values of λ (right hand scale) and T_c (left hand scale). In each case the lower curves refer to La_2CuO_4 (i.e. stars and diamonds) and the upper curves (triangles and squares) refer to $La_{1.86}(Ba,Sr)_{0.14}CuO_4$.

Table I. Densities of states at E_F (states/eV/spin), electron-ion matrix element $\langle I^2 \rangle$ (eV/A)^2 and McMillan-Hopfield parameter η (eV/A^2) per atom, and the total η for all O atoms in the cell. For the $LaBaCuO_4$ compound, the La and Ba quantities have been averaged.

	La_2CuO_4	$La_{1.86}Ba_{0.14}CuO_4$	$LaBaCuO_4$	$LaCuO_3$	$BaCuO_3$	$CsCuO_3$
$N(E_F)$	0.62	1.08	1.85	0.71	1.35	3.48
$\langle I_2 \rangle_{La,Ba,Cs}$	0.0	0.006	0.07	0.0	0.009	0.14
$\langle I^2 \rangle_{Cu}$	1.00	0.69	0.59	1.25	1.22	0.24
$\langle I^2 \rangle_{O_{xy}}$	1.16	0.94	0.17	0.68	0.44	0.15
$\langle I^2 \rangle_{O_z}$	0.06	0.10	0.13	-	-	-
$\eta_{La,Ba,Cs}$	0.0	0.006	0.12	0.0	0.012	0.49
η_{Cu}	0.62	0.74	1.08	0.89	1.65	0.82
$\eta_{O_{xy}}$	0.72	1.00	0.32	0.48	0.60	0.51
η_{O_z}	0.04	0.10	0.24	-	-	-
$\eta_{O_{tot}}$	1.52	2.20	1.12	1.44	1.80	1.53