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Composition dependence of transition temperature in new superconductors: $La_{2-x}(Ba, Sr)_xCuO_4$

R K SINGH[†], A C SHARMA*, N K GAUR and DINESH VARSHNEY
School of Physics, Barkatullah University, Bhopal 462026, India
*School of Studies in Physics, Jiwaji University, Gwalior 474011, India

Abstract. We have investigated the variation of transition-temperature and coupling parameter with the composition concentration in $La_{2-x}(Ba, Sr)_xCuO_4$ superconductors using a formulation developed on the basis of an idea of pairing of charge carriers by exchange of both acoustic plasmons and phonons. Reasonably good agreement is found between the recent experimental results and our theoretical results on the superconducting transition temperature.

Keywords. Superconductors; plasmons; phonons; transition temperature; coupling parameter.

1. Introduction

The study of composition (x) dependence of the transition temperature (T_c) in La_{2-x} $(Ba, Sr)_x$ CuO_4 and other La_2CuO_4-based superconductors has become a subject of increasing interest (Bednorz *et al* 1987; Dover *et al* 1987; Moodenbaugh *et al* 1988; Markert *et al* 1988) since the discovery of high T_c in them (Markert *et al* 1988). Recently, Dove *et al* (1987) measured T_c as a function of x in $La_{2-x}Sr_xCuO_4$ system and found that T_c first increases and then decreases with x after reaching its maximum value at $x = 0{\cdot}15$. Also they found that for $x < 0{\cdot}06$, T_c is almost zero. More recently, Moodenbaugh *et al* (1988) observed similar variation of T_c with x in $La_{2-x}Ba_xCuO_4$ system with T_c having two maxima values at $x = 0{\cdot}09$ and $x = 0{\cdot}15$. Bednorz *et al* (1987) and Markert *et al* (1988) also reported similar behaviour of T_c as a function of x in $La_{2-x}Ca_xCuO_4$ and $La_{2-x}Na_xCuO_4$ systems. Motivated by these experimental observations, we thought it pertinent to present a theoretical analysis of T_c as a function of x.

The variation of x in La_2CuO_4-based superconductors can introduce two types of changes in the system. The first is the change in carrier states and free carrier density n_c and the second is the change in crystal structure. The usual bulk properties are not expected to change significantly for small variations in x. Therefore one cannot expect that BCS type theory, based on the pairing of charge carriers by exchange of phonons only, can satisfactorily explain the drastic change in T_c as a function of x. This, in turn, suggests the involvement of carrier (hole) excitations along with phonons in pairing of current carrying charge carriers. Electronic excitation such as ordinary plasmons, whose energy is comparable with the Fermi energy, cannot participate in pairing mechanism because of strong scattering effects near the Fermi

[†]For correspondence

surface. One therefore can accept an involvement of acoustic plasmons, whose energy is much smaller than the Fermi-energy in pairing mechanism.

Considering the layered structure of La_2CuO_4-based superconductors, one can calculate the frequencies of collective excitations in these systems. One finds a well-defined two-dimensional (2D) acoustic plasmon branches. The cut-off plasmon frequency is much larger than the Debye frequency. Keeping this in mind, we have calculated T_c as a function of x using the formalism based on the assumption of charge carrier pairing by exchange of both 2D acoustic plasmons and phonons in La_2CuO_4-based superconductors. This takes care of change in n_c and carrier states on changing x.

The effect of change in crystal structure on varying x can partially be taken into account by introducing the x-dependence of the background dielectric constant ε. We express ε as a function of x with perfect lattice approximation. We have computed T_c as a function of x for $La_{2-x}(Ba,Sr)_xCuO_4$ system. Considering a quasi-2D nature of charge carriers, our calculations are compared with recent experimental result (Dover *et al* 1987; Moodenbaugh *et al* 1988).

2. Formalism

By incorporating the effects of pairing of the charge carriers by exchange of both 2D acoustic plasmons and the phonons within the BCS framework, T_c can be written as (Kresin 1987)

$$T_c = T_c^{\text{ph}} (\omega_{pl}/T_c^{\text{ph}})^h \tag{1}$$

where T_c^{ph} is the contribution due to the phonon-pairing mechanisms and is given by

$$T_c^{\text{ph}} = 1{\cdot}14\,\omega_{\text{ph}} \exp[-(1+\lambda_{\text{ph}})/\lambda_{\text{ph}}] \tag{2}$$

The abbreviation h in (1) stands for

$$h = \lambda_{\text{pl}}/(\lambda_{\text{pl}} + \lambda_{\text{ph}}) \tag{3}$$

with ω_{ph} (ω_{pl}) and λ_{ph} (λ_{pl}) as the frequency and coupling parameters for phonons (plasmons).

The x-dependence of T_c^{ph} and λ_{ph} are found to be more significant for $x > 0{\cdot}15$ (Weber *et al* 1987). The x dependence of T_c is introduced via the x-dependence of ω_{pl}, λ_{pl} and T_c^{ph}. Considering the 2D-nature of the charge carriers, λ_{pl} and ω_{pl} can be written as (Kresin 1987)

$$\lambda_{\text{pl}} = m^* e^2/[\varepsilon \hbar^2 (2\pi n_c)^{1/2}] \tag{4}$$

and

$$\omega_{\text{pl}} = (\hbar^2 \pi n_c/m^* \varepsilon)\sqrt{\lambda_{\text{pl}}} \tag{5}$$

with $\hbar(=h/2\pi)$ as the Planck's constant.

To introduce the x-dependence in λ_{pl} and ω_{pl}, we have assumed the linear variation of n_c and ε with x for small values of x such that

$$\varepsilon = (2-x)\varepsilon_\infty(La_2CuO_4) + x\varepsilon_\infty(Ba,Sr)CuO_4. \tag{6}$$

The results of calculations have been presented and discussed below.

3. Results and discussion

We have computed λ_{pl} and ω_{pl} from (4) and (5) using (6) for various values of x starting from $x = 0{\cdot}01$ to $x = 0{\cdot}25$ in $La_{2-x}Ba_xCuO_4$ and $x = 0{\cdot}01$ to $x = 0{\cdot}5$ in $La_{2-x}Sr_xCuO_4$ systems. The parameters involved in our calculations of λ_{pl} and of ω_{pl} are taken as follows:

$$n_0 = 2{\cdot}52 \times 10^{14}\,\text{cm}^{-2},$$

$$m^* = 2m_e \text{ (for } La_{2-x}Ba_xCuO_4\text{)},$$

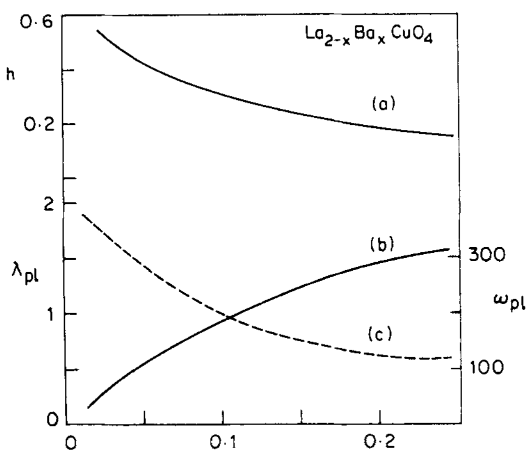
and $$m^* = m_e \text{ (for } La_{2-x}Sr_xCuO_4\text{)},$$

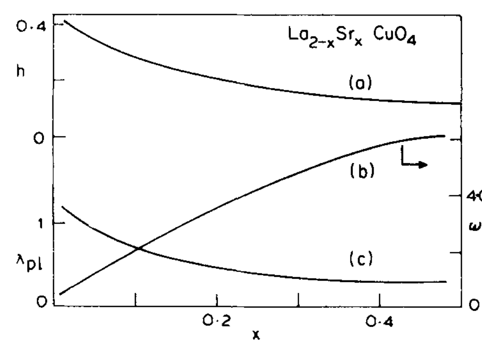
where m_e is the bare electron mass. The values of ε_∞ $(La_2CuO_4) = 10$ and ε_∞(Ba, Sr) $CuO_4 = (4, 3)$ are arbitrarily chosen. However, they are supposed to be in the correct range of experimental values of dielectric constants of various insulators and semiconductors. We have also calculated coupling parameter h for various x values taking $\lambda_{ph} = 1{\cdot}5$ (Weber *et al* 1987).

A plot of our calculated values of λ_{pl}, h and ω_{pl} against x is shown in figures 1 and 2 for $La_{2-x}Ba_xCuO_4$ and $La_{2-x}Sr_xCuO_4$. It is seen from these figures that the values of λ_{pl} and h decrease while the values of ω_{pl} increase with the increase of x.

Using these values of h, ω_{pl}, T_c^{ph} and λ_{ph} for various x values, we computed T_c as a function of x. Our computed values of T_c are plotted as a function of x in figures 3 and 4 along with the experimental values. These figures show an overall agreement between our calculated values of T_c and the available experimental data (Dover *et al* 1987; Moodenbaugh *et al* 1988). It is found that in $La_{2-x}Ba_xCuO_4$, there are two maxima, both at $T_c = 27$ K near composition $x = 0{\cdot}10$ and $0{\cdot}15$ with the corresponding two measured peaks (Moodenbaugh *et al* 1988) near $x = 0{\cdot}09$ and $x = 0{\cdot}15$ at $T_c = 25$ K and in $La_{2-x}Sr_xCuO_4$ there is one peak at $T_c = 41$ K near $x = 0{\cdot}15$ with corresponding peak measured (Dover *et al* 1987) at $T_c = 43{\cdot}5$ K near $x = 0{\cdot}15$.

We have found that our simple calculation, based on the mechanism of pairing of





Figures 1 and 2. Variation of the parameters: h ω_{pl} and λ_{pl} with x. **1.** $La_{2-x}Ba_xCuO_4$ and **2.** $La_{2-x}Sr_xCuO_4$.

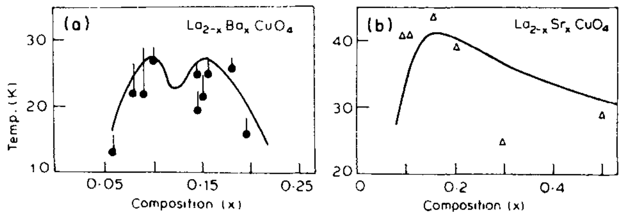


Figure 3. Variation of T_c with x. **a.** The circles (Φ) are the experimental data taken from Moodenbaugh *et al* (1988). **b.** The triangles (Δ) are the mid-points of the error bars from Dover *et al* (1987).

charge carriers by exchange of both acoustic plasmons and phonons, explains satisfactorily the experimental behaviour of T_c as a function of x.

Thus, we may conclude that other theoretical attempts, based on the calculation of T_c contributed only from the pairing of charge carriers by exchange of phonons are not able to predict the observed trend of variation of T_c over the entire range of x (Weber *et al* 1987). It is therefore obvious that the role of electronic excitations is also important in describing T_c in $La_{2-x}(Ba,Sr)_xCuO_4$ and other related ceramic superconductors. It is seen that for $0{\cdot}06 < x < 0{\cdot}15$, the mechanism of electronic excitations is dominant over phonon mechanism, while for $x > 0{\cdot}15$, the phonon mechanism is dominant over the electronic excitations. In order to introduce further improvement in the agreement between the experimental and our theoretical results on T_c in $La_{2-x}(Ba,Sr)_xCuO_4$ and other ceramic superconductors, our formulation can be modified in the following way:

The method used for calculation of T_c in this paper does not take proper account of the appropriate acoustic plasmon dispersion, which corresponds to the actual La_2CuO_4-based superconducting systems. By taking an appropriate account of the acoustic plasmon dispersion, a modified form of x-dependent T_c can be obtained (Sharma 1989). We have planned to introduce these modifications in our future study.

In conclusion, we have presented a simple calculation of T_c as a function of x for $La_{2-x}(Ba,Sr)_xCuO_4$ superconductors. Our results show a reasonably good agreement with experimental data on T_c reported by others. Also, we have demonstrated that the carrier collective excitations (like plasmons) play an important role in pairing of charge carriers. This conclusion is in keeping with the earlier study of one of us (Sharma 1989) in the case of copper oxide superconductors.

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