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1999 J. Phys.: Condens. Matter 11 4401

(http://iopscience.iop.org/0953-8984/11/22/311)

J. Phys.: Condens. Matter **11** (1999) 4401–4407. Printed in the UK PII: S0953-8984(99)00680-3

Pressure dependence of T_c for $La_{2-x}Sr_xCuO_4$ as a function of carrier concentration

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Received 6 January 1999, in final form 16 March 1999

Abstract. The pressure effect on T_c for $La_{2-x}Sr_xCuO_4$ has been investigated within the van Hove singularity scenario of high-T_c superconductivity by taking into account the variation of the Fermi energy and the effective attractive interaction with pressure. It was found that the pressure coefficient of T_c decreases with increasing T_c and remains positive over the whole doping region. The predicted T_c increases with increasing pressure, reaching a maximum at 4 GPa, and then decreases with further increasing pressure. These results are in agreement with experiments.

1. Introduction

High-pressure studies have been shown [1–3] to be effective in elucidating the microscopic mechanism of the superconducting state and in providing clues that are useful in the search for new ground states of solids as well as in finding new materials with higher critical temperatures by using the chemical pressure. $La_{2-x}Sr_xCuO_4$ is the simplest superconducting cuprate system in that it has a single CuO_2 conducting layer and in that the hole concentration in the CuO_2 plane is uniquely determined by the Sr concentration in the La(Sr)O double layers. The pressure effect on the superconducting transition temperature T_c in $La_{2-x}Sr_xCuO_4$ compounds has attracted particular interest because the pressure coefficient, $\mathrm{d}\ln T_c/\mathrm{d}P$, is positive over the whole doping range [4–6], which contrasts with the decrease in T_c under pressure observed in the overdoped region for other single-Cu–O-layer cuprates, $Tl_2Ba_2CuO_{6+y}$ [7] and $HgBa_2CuO_{4+\delta}$ [8]. Meanwhile, the pressure derivative of T_c, $\mathrm{d}T_c/\mathrm{d}P$, is very high compared with those for other hole-doped high-T_c superconductors (HTSCs). On the other hand, the $La_{2-x}Sr_xCuO_4$ system shows the nonlinear pressure dependence of T_c [4, 6] generally found for HTSCs. Within the pressure-induced charge-transfer model (PICT) [9–11], $\mathrm{d}T_c/\mathrm{d}P$ is expected to depend strongly on the carrier concentration in the CuO_2 planes. The always-positive $\mathrm{d}T_c/\mathrm{d}P$ values found for $La_{2-x}Sr_xCuO_4$, irrespective of the doping level, go against this simple model. So far, there have been few successful theoretical analyses of the pressure dependence of T_c in this system.

With the aim of establishing the origin of the high critical temperature and the anomalous normal-state properties of HTSCs, several models have been proposed. The van Hove

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0953-8984/99/224401+07$19.50

singularity (VHS) scenario is one such model, based on the phonon-mediated BCS pairing mechanism. The anomalous isotope effect, the linear temperature dependence of the resistivity, the pressure effect, and some characteristic features of the thermoelectric power of the high-T_c oxides can be explained qualitatively within the VHS scenario [12,13]. High-resolution angle-resolved photoemission data have identified the presence of a saddle point in the band-structure energy surface within 100–200 K of the Fermi energy (E_F) [14, 15]. The electrostatics of the system will be changed under the application of pressure, which causes a charge redistribution to take place in such a way that the carrier concentration (n_H) in the CuO_2 plane changes. Such an effect has been observed in Hall effect [16], thermopower [17], and neutron power diffraction [18] investigations under high pressure. Electronic structure calculations [19] indicate that there is a prominent VHS close to the Fermi energy E_F and that the behaviour of T_c depends strongly on the Fermi level passing close to or through the energy location of the VHS with increasing pressure, and also that there is a correspondence between the hole doping and the pressure treatment. Hence, E_F can be viewed as a pressure-sensitive variable.

Previous studies suggested that interlayer coupling between the adjacent CuO_2 layers plays an important role in enhancing T_c [20–24]. The origin of the interlayer coupling has been found to be the addition of interlayer interaction [25]. Furthermore, Tesanovic [26] found that the interlayer coupling due to interactions plays an important role both in stabilizing the long-range order in cuprate superconductors and in providing a mechanism for further enhancement of T_c. It has been proposed that the enhancement of T_c with pressure also arises through a gradual increase of the pressure-induced interlayer coupling [27, 28]. Using high-pressure Raman scattering, Aronson *et al* [29] found that the in-plane superexchange interaction J in antiferromagnetic La_2CuO_4 varies with pressure, which is directly related to the effective pairing interaction V_{eff}. It is reasonable to assume that the pressure-induced change of V_{eff} is another important factor in producing the pressure dependence of T_c.

In this paper, we provide a theoretical explanation for the pressure effect on T_c in the typical compound $La_{2-x}Sr_xCuO_4$ in terms of the VHS scenario within the BCS framework [12,30], in which (i) the difference between the Fermi energy E_F and E_{VHS} and (ii) the effective pairing interaction V_{eff} are considered to be the two pressure-dependent variables.

2. Theoretical approach

The quasiparticle energy in a tight-binding band is given by

$$E(\vec{k}) = -2t(\cos k_x a + \cos k_y a) + 4t_2 \cos k_x a \cos k_y a \tag{1}$$

where a is the lattice spacing between Cu atoms on the (x, y) plane, and t and t_2 are the nearest-neighbour and the next-nearest-neighbour hopping integrals, respectively.

The density of states per spin is easily calculated as

$$N(E) = N_0 \ln \left| \frac{D}{E - E_F + \delta} \right|. \tag{2}$$

Here $D = 16t(1-4t_2^2/t^2)^{1/2}$, $N_0 = 8/(\pi^2 D)$ is the density of states normalized to a flat band, $\delta = E_F - E_{VHS}$, and $E_{VHS} = -4t_2$ is the energy at which the VHS is located. In high-T_c superconductors the Fermi level (E_F) shifts with doping, and correspondingly δ changes. The equation for the superconducting transition temperature T_c, obtained from the standard BCS gap equation, is

$$\frac{2}{V_{eff}} = \int_{E_F-\omega_D}^{E_F+\omega_D} N(E) \tanh \frac{E - E_F}{2T_c} \frac{\mathrm{d}E}{E - E_F} \tag{3}$$

where V_{eff} is an effective interaction due to exchange of phonons, spin fluctuations, or combined charge fluctuations and lattice distortions, and ω_D is the cut-off energy. In order to generalize equation (3) to include the effects of pressure, we assume that the pressure dependence of the parameters D and ω_D can be neglected to a first approximation. Thus the pressure dependence of the intrinsic T_c in equation (3) is related to the pressure dependence of the parameters δ and V_{eff}. That is,

$$\delta(P) = \delta + a_1 P \tag{4}$$

and

$$V_{eff}(P) = V_{eff}(1 + a_2 P) \tag{5}$$

where $a_1 = \mathrm{d}\delta/\mathrm{d}P|_{P=0} \propto \delta\kappa_V$ [31], $a_2 = \mathrm{d}\ln V_{eff}/\mathrm{d}P|_{P=0} = -\kappa_V\,\mathrm{d}\ln V_{eff}/\mathrm{d}\ln V|_{P=0}$, and $\kappa_V = -\mathrm{d}\ln V/\mathrm{d}P|_{P=0}$ is the volume compressibility. This approximation is reasonable for low values of P, but is likely to break down for large P since one expects $V_{eff}(P)$ and $\delta(P)$ to saturate at larger pressures. Thus the variation of T_c with pressure P can be simply written as

$$T_c(P) = T_c[\delta(P), V_{eff}(P)]. \tag{6}$$

From equations (3) and (6) one can calculate $\mathrm{d}T_c(P)/\mathrm{d}P$ as

$$\frac{\mathrm{d}T_c(P)}{\mathrm{d}P} = \frac{1}{I(P)}\frac{4a_2V_{eff}}{N_0(V_{eff}(P))^2} - \frac{2a_1}{I(P)}\int_{E_F-\omega_D}^{E_F+\omega_D}\tanh\frac{E-E_F}{2T_c(P)}\frac{1}{E-E_F+\delta(P)}\,\frac{\mathrm{d}E}{E-E_F} \tag{7}$$

with

$$I(P) = \int_{E_F-\omega_D}^{E_F+\omega_D}\frac{1}{(T_c(P))^2}\ln\left|\frac{D}{E-E_F+\delta(P)}\right|\mathrm{sech}^2\left(\frac{E-E_F}{2T_c(P)}\right)\mathrm{d}E. \tag{8}$$

Putting $P = 0$, one can obtain the initial pressure coefficient of T_c, $\mathrm{d}\ln T_c/\mathrm{d}P$, as

$$\frac{\mathrm{d}\ln T_c}{\mathrm{d}P} = \frac{1}{T_cI(0)}\frac{4a_2}{N_0V_{eff}} - \frac{2a_1}{T_cI(0)}\int_{E_F-\omega_D}^{E_F+\omega_D}\tanh\frac{E-E_F}{2T_c}\frac{1}{E-E_F+\delta}\,\frac{\mathrm{d}E}{E-E_F}. \tag{9}$$

From equations (6) and (7), one notices that in order to study the pressure dependence of $T_c(P)$ and $\mathrm{d}T_c(P)/\mathrm{d}P$, one must have a knowledge of the values of a_1 and a_2. In general, the Fermi level shifts toward the energy location where the VHS lies under the application of pressure for underdoped materials and overdoped materials. The sign of $\mathrm{d}\delta/\mathrm{d}P$ is then expected to be positive for underdoped compounds and negative for overdoped compounds. It is therefore reasonable to write $a_1/\omega_D = -\beta\delta\kappa_V$ where β is a constant which depends on the superconducting material. In the present study we consider the value of β of 0.1 for the $La_{2-x}Sr_xCuO_4$ system.

The success of the VHS scenario lies in the assumption that δ is zero for the optimum doping concentration for which T_c is maximum [12]. When the compound is optimally doped, $\delta = 0$ and thus $a_1 = 0$. Putting these values into equations (3) and (9), one can obtain an expression for a_2:

$$a_2 = \frac{1}{2T_c^{\max}}\frac{\mathrm{d}\ln T_c^{\max}}{\mathrm{d}P}\left[\int_{E_F-\omega_D}^{E_F+\omega_D}\ln\left|\frac{D}{E-E_F}\right|\mathrm{sech}^2\left(\frac{E-E_F}{2T_c^{\max}}\right)\mathrm{d}E\right] \times\left[\int_{E_F-\omega_D}^{E_F+\omega_D}\ln\left|\frac{D}{E-E_F}\right|\tanh\left(\frac{E-E_F}{2T_c^{\max}}\right)\frac{\mathrm{d}E}{E-E_F}\right]^{-1}. \tag{10}$$

Therefore the values of a_2 as well as $\mathrm{d}\ln V_{eff}/\mathrm{d}\ln V|_{P=0}$ for HTSCs can be determined from equation (10) on the basis of the experiment values of $T_c^{\max}$ and $\mathrm{d}T_c^{\max}/\mathrm{d}P$.

3. Results and discussion

For fixed values of the parameters D and ω_D and of the pairing potential V_{eff}, equation (3) yields the solutions for T_c. According to equation (3), we plot the transition temperature in figure 1 as a function of the position of the Fermi level with respect to the van Hove singularity with different values of V_{eff}. The parameters used in the numerical calculation are $D = 5800$ K and $\omega_D = 754$ K [12]. It is seen that transition temperature peaks extremely strongly around the point where the Fermi level lies at the saddle point. T_c is maximum at $\delta = 0$ and decreases as $|\delta|$ increases, i.e., as the Fermi level shifts from the energy of the VHS. On the other hand, the transition temperature increases with the increase of V_{eff}. When $\delta \to 0$ the transition temperature rises rapidly with V_{eff}. In fact, the variation in the transition temperature among the various cuprate superconductors indicates that T_c should be related to V_{eff} [32]. The magnitude of T_c depends strongly on the doping level x and reaches its maximum at $x \simeq 0.16$ in the $La_{2-x}Sr_xCuO_4$ system [33]. The change in T_c with composition x is associated with a change of δ through E_F. These results are very consistent with the present picture. Thus, it is clear that the strong variation in $N(E_F)$, derived from the quasi-2D VHS, plays a dominant role in the anomalous behaviour of T_c with varying composition x in $La_{2-x}Sr_xCuO_4$.

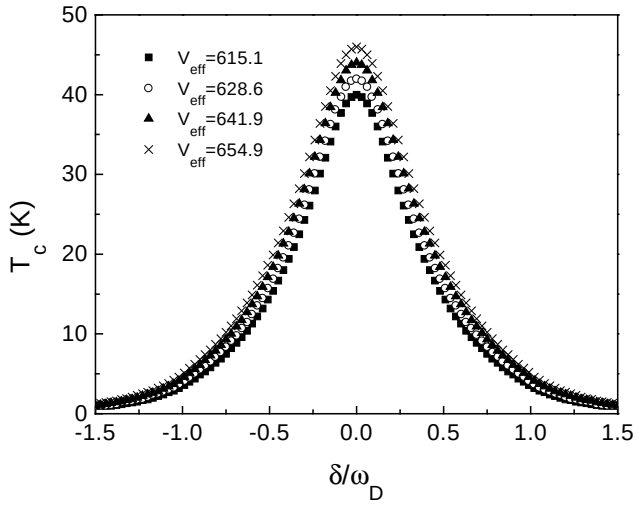

Figure 1. Variation of the superconducting transition temperature T_c with δ/ω_D for different coupling parameters: squares: $V_{eff} = 615.1$; open circles: $V_{eff} = 628.6$; upwards-pointing triangles: $V_{eff} = 641.9$; crosses: $V_{eff} = 654.9$. $D = 5800$ K, $\omega_D = 754$ K.

The above analysis enables us to plot $\mathrm{d}\ln T_c/\mathrm{d}P$ as a function of δ. For the $La_{2-x}Sr_xCuO_4$ systems, the maximum T_c of 39 K, the maximum pressure derivative $\mathrm{d}T_c^{\max}/\mathrm{d}P$ of 3.1 K GPa^{-1} [5], and the volume compressibility κ_V of 6.8×10^{-3} GPa^{-1} [34] are obtained when the compound is optimally doped. With these parameters, equation (10) yields a value of $\mathrm{d}\ln V_{eff}/\mathrm{d}\ln V|_{P=0}$ of about -5.0. Then the pressure coefficient $\mathrm{d}\ln T_c/\mathrm{d}P$ can be calculated numerically by using equation (9). The variation of both T_c and $\mathrm{d}\ln T_c/\mathrm{d}P$ with δ for $La_{2-x}Sr_xCuO_4$ is shown in figure 2. For comparison, data from Tanahashi *et al* [5] are also displayed. The curves for T_c and $\mathrm{d}\ln T_c/\mathrm{d}P$ as functions of δ show the typical shape observed experimentally. The pressure coefficient is larger for underdoped samples (negative δ) than at optimum doping ($\delta \sim 0$). The minimum $\mathrm{d}\ln T_c/\mathrm{d}P$ occurs in the overdoped region (positive δ). It is interesting to note that $\mathrm{d}\ln T_c/\mathrm{d}P$ is positive for all values of δ, in agreement with

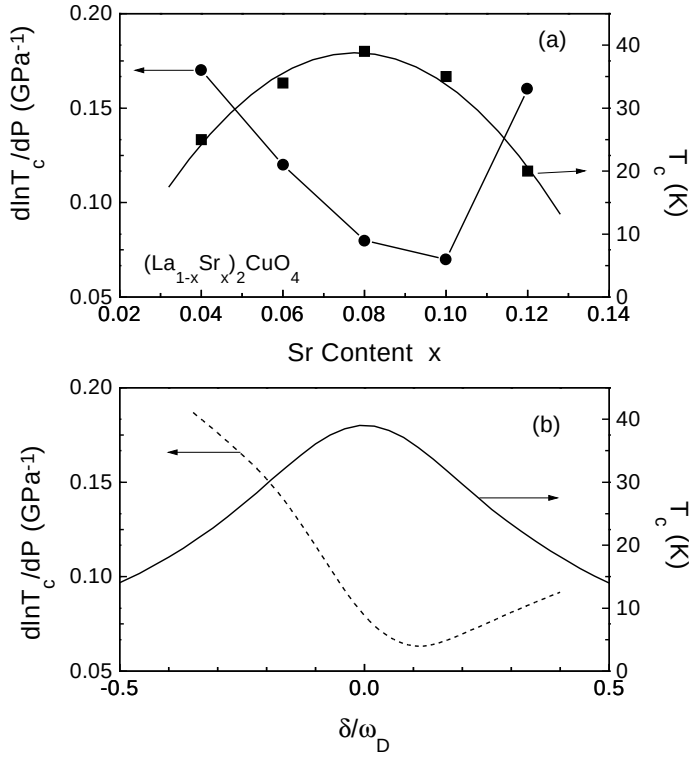

Figure 2. (a) Experimental values, taken from the work of Môri *et al* [6] for the superconducting transition temperature T_c and the pressure coefficient $\mathrm{d}\ln T_c/\mathrm{d}P$ of $La_{2-x}Sr_xCuO_4$ as functions of x. (b) Calculated values of T_c and $\mathrm{d}\ln T_c/\mathrm{d}P$ versus δ/ω_D.

observation [5]. Similar behaviour has been reported by Jansen *et al* [35] on the basis of an indirect exchange pairing mechanism for conduction electrons via oxygen anions.

The procedure developed above is now applied to a numerical evaluation of $T_c(P)$ for the nearly optimally doped but slightly underdoped $La_{2-x}Sr_xCuO_4$ compound with $T_c = 36.6$ K. The corresponding value of δ can be determined from equation (3) as $\delta/\omega_D = -9.0 \times 10^{-2}$. Hence one obtains $a_1/\omega_D = 6.12 \times 10^{-2}$. On the basis of these parameters, we calculated T_c from equation (6) as a function of pressure P in the range $0 \leqslant P \leqslant 8$ GPa. In figure 3 we present the numerical results. As can be seen, as pressure is increased, T_c increases initially until it reaches a maximum at some pressure level, and at higher pressures T_c decreases. The maximum T_c of 46 K on the T_c–P curve is exhibited at about 4 GPa. The hydrostatic pressure study by Môri *et al* [6] shows that $T_c(P)$ passes through a maximum at 4 GPa. Erskine *et al* [4] found a gradual increase of T_c with pressure up to ∼4 GPa, a plateau of 46 K from 4 to 6 GPa and a decrease above 6 GPa. Interestingly, our prediction coincides well with experiments. The predicted variation of T_c with pressure in $La_{2-x}Sr_xCuO_4$ is very similar to that found for $YBa_2Cu_3O_{7-\delta}$ and Hg-based series within the framework of the PICT model [9, 10]. It is therefore indicated that the VHS scenario can account for the pressure effect on T_c in hole-doped HTSCs.

The present VHS scenario is based on the assumption of s-wave pairing. However, recent experiments seem to increasingly favour d-wave, in particular $d_{x^2-y^2}$, pairing. Recently, Newns *et al* [36] investigated the assumption that the pairing has $d_{x^2-y^2}$ symmetry in an investigation

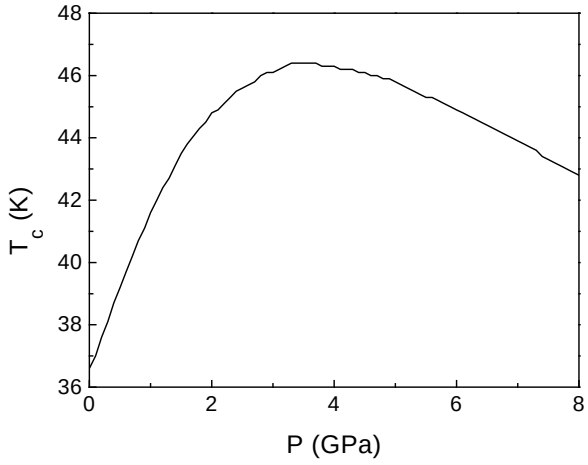

Figure 3. The pressure dependence of T_c in the nearly optimally doped but slightly underdoped $La_{2-x}Sr_xCuO_4$ compound with $T_c = 36.6$ K up to 8 GPa.

of the transition temperature, gap, and specific jump at the BCS level of approximation. It is found that the effect of the VHS on these properties is similar to the effect of s-wave pairing. In particular, the two intrinsic factors which are responsible for the value of T_c under pressure are the same, i.e., T_c decreases with the increase of $|\delta|$ and reaches the maximum value when $\delta = 0$; meanwhile T_c increases with the effective coupling constant V_{eff}. Therefore, it is indicated that considering the VHS scenario with d-wave pairing would not make much difference from considering the case with s-wave pairing as regards the pressure dependence of T_c, at least qualitatively.

4. Conclusions

We have investigated the pressure dependence of the superconducting transition temperature for the typical cuprate superconductors $La_{2-x}Sr_xCuO_4$ in terms of the van Hove singularity scenario. The model utilized the assumption that both (i) the difference between the Fermi level and the van Hove singularity and (ii) the pairing potential change under the application of pressure can account for the pressure dependence of T_c observed experimentally. The pressure coefficients of T_c are observed to be positive for all dopant concentrations x. The predicted T_c is found to increase with increasing pressures, reaching a maximum at 4 GPa, and then decrease with further increasing pressure. These results are in agreement with experiments. Thus, this analysis suggests that a reasonable description of the pressure dependence of T_c for the $La_{2-x}Sr_xCuO_4$ cuprates can be realized using an s-wave theory for T_c.

Acknowledgments

The work was supported by the China Postdoctoral Science Foundation and in part by the Centre for Research and Development on Superconductivity of China.

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