



On the Critical Temperature of Superconductivity of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ Thin Films

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Abstract

Superconductivity of the cuprate $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ thin films is considered within the concept of the preformed pairs (bipolarons). Taking the extended Holstein-Hubbard model as a basis for a strongly interacting hole-lattice system of the cuprate films, a relation between the temperature of Bose-Einstein condensation (T_{BEC}) of an ideal gas of the intersite bipolarons and the strains in the thin films is established. In doing that (relation), the chain model of cuprates, proposed by Alexandrov and Kornilovitch in ref. (Phys Rev Lett 82(4):807, 1999), is used. It is shown that the calculated values of the temperature of Bose-Einstein condensation of the bipolarons in the cuprate $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ thin films grown on LaSrAlO_4 and SrTiO_3 substrates correlate (and at certain values of doping level x satisfactorily agree) with the experimental values of the critical temperature of superconductivity (T_c) of the above systems. The T_{BEC} versus x dependence obtained within the approach is very similar to the dome-shape type T_c versus x phase diagram of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ thin films. The obtained phase diagram has a feature of “1/8”-anomaly which is a common for both bulk and film samples of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$.

Keywords Cuprate thin films · Uniaxial strain · Bipolaronic superconductivity · Bose-Einstein condensation

1 Introduction

Despite the intensive experimental and theoretical studies, for almost four decades now, the mechanism of high- T_c superconductivity of the cuprates remains not entirely clear. Although, a huge amount of experimental data has been accumulated so far on various aspects of the phenomenon,

there is no theoretical understanding of these data within the framework of a single concept [2]. The existing theoretical models are unable to explain all aspects of high- T_c superconductivity of cuprates. Even the high- T_c superconductivity of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO) cuprate with the simplest crystal structure is not fully understood, although there is progress in understanding of some particular aspects of this complex phenomenon. One may say that LSCO cuprate is a testing playground for the models of high- T_c superconductivity. The same is true for thin films of LSCO cuprate whose superconducting properties differ from that of bulk counterparts [3].

Study of superconducting properties of the LSCO thin films was started by the works [4–7]. Since then, a number of papers have been published on the superconductivity of the LSCO thin films [8–21]. A more detailed information about the recent achievements in the field of superconductivity of the LSCO thin films can be found in the review [3]. The main conclusion of the works [8–21] is that the superconductivity of LSCO thin films depends on several factors. These factors, in addition to the doping level (x), include the growing and annealing conditions of the thin films, the thickness of the thin film itself, and the type of substrate for the thin film. All of the above factors affect the properties of the thin films, determining, in particular, the value of its

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critical temperature of superconductivity (T_c). Early studies showed that T_c of LSCO thin films depends, at constant doping level and under the same thin film growth conditions, on the strains induced by lattice mismatch between the film and the substrate. It was established that for the (001) oriented thin film of LSCO the compressive strain of the *ab*-plane lattice constants enhances T_c while the compressive strain of the lattice period along *c*-direction reduces T_c [9]. Two substrates are often used for the LSCO thin film growth. They are LaSrAlO₄ (LSAO) and SrTiO₃ (STO) with the lattice periods of 3.756 Å and 3.905 Å, respectively. It turns out that for the LSCO thin film grown on LSAO (STO) substrate the *ab*-plane periods are compressed (elongated) and the period in the perpendicular *c*-direction is elongated (compressed). While a research community has a common view of point of the reasons of enhancement and/or reduction of T_c of the thin films which is due to the structural changes of the lattice constants of the film, it is worth to do some notes on the issue. First of all, one must recognize that the study of superconducting properties of the cuprate thin films, in particular LSCO thin films, has become actual due to the possibility of the potential application of the cuprate thin films in the different superconducting devices [22–25]. Secondly, there are conflicting quantitative reports on the values of T_c of the LSCO thin films obtained at the different doping levels, film thicknesses and other conditions [3, 10, 13]. Thirdly, in the literature, one may come to across to the variety of qualitative approaches (theoretical models) to the strain(pressure)-induced high- T_c phenomena in the LSCO thin films [11, 26–29].

Although these models claim to be able to explain the numerical values of T_c of the LSCO thin films, one cannot say that they take into account all features of the phenomenon under consideration. This concerns the role of the electron-phonon interaction (EPI) in the cuprates which implies a possibility of polaron/bipolaron formation in the strong coupling limit, while quasiparticle tunneling spectra study of La_{1.84}Sr_{0.16}CuO₄ films gave clear evidence that the phonons are the relevant bosons involved in quasiparticle-boson interactions [17]. In addition, in the above papers, the phenomenon is considered as a purely two-dimensional one. While the cuprates have a quasi-two-dimensional crystal structure, it is well understood that EPI plays an important role in the cuprates [30, 31], in particular, EPI that involves *apical* oxygen atoms determines dynamics of charge carrier in copper-oxygen (CuO₂) plane [32]. And EPI is strong enough for favouring (bi)polaron formation [33]. The strong EPI manifests itself as polaronic nature of charge carriers in the cuprates [34]. The results of many experiments are also in satisfactory agreement with a (bi)polaronic approach to cuprate superconductivity [35–37]. One may conclude that the above theoretical models consider the LSCO thin films totally ignoring the strong electron-phonon interaction,

and consequently ignoring the possibility of polaron and/or bipolaron formation. They ignore, in particular, the interaction of in-plane (CuO₂) charge carriers with the *c*-polarized vibrations of the apex oxygen atoms. The latter interaction, which depends mainly on the apical-oxygen displacements, as shows an improved X-ray phase-retrieval method study has a profound effect on the value of T_c of LSCO thin films [38]. Therefore, a systematic and comprehensive study of the dependence of the value of T_c of LSCO thin films, grown on various families of substrates, on doping level *x* (or Sr concentration) is of considerable importance for understanding the occurrence of superconductivity not only in these materials but also, in general, in whole family of the cuprates.

In this work, we will try to consider the issue of high- T_c superconductivity of the LSCO thin films, taking into account the polaronic features of the phenomenon. In doing this, we rely on the extended Holstein-Hubbard (or Fröhlich-Coulomb) model of high- T_c superconductivity which assumes formation of intersite bipolarons and their Bose-Einstein condensation (BEC) giving rise the superconductivity. The main idea of our approach was given early in the works [39, 40]. In the work [39], the values of T_c of La_{1.85}Sr_{0.15}CuO₄ and La_{1.9}Sr_{0.1}CuO₄ thin films, grown on LSAO and STO substrates, were satisfactorily explained. The work [40] extends our approach to RBa₂Cu₃O_{7- δ} cuprates. Here, we will try to explain the dependence of the value of T_c of LSCO thin films, grown on LSAO and STO substrates, on doping level *x* (or Sr concentration).

2 The Model

The cuprates are characterized as a strongly correlated electron (or hole) and strongly coupled electron-phonon system. Such the system can be described by means of an extended Holstein-Hubbard (or Fröhlich-Coulomb) model [41]. It was shown that within the model, at strong EPI regime and nonadiabatic approximation, intersite bipolaron tunnel in the first order of polaron tunneling and its mass has the same order as polaron mass. For the sake of simplicity, we suppose that the intersite bipolarons form an ideal gas of charged carriers and mass of bipolaron is twice of polaron's mass, i.e. $m_{bp} = 2m_p$. Then, the temperature of Bose-Einstein condensation of the intersite bipolarons defines as [39, 40]

$$T_{BEC} = \frac{3.31\hbar^2 n^{2/3}}{2k_B m^*} e^{-g^2}, \quad (1)$$

where \hbar (k_B) is Planck's (Boltzmann's) constant, $m^* = \hbar^2/2t(a)^2$ is the bare band mass, n is density of the intersite bipolarons and g^2 is the mass renormalization factor of polaronic system. In order to get expression for g^2 , one uses a chain model lattice (Fig. 1) that was introduced by

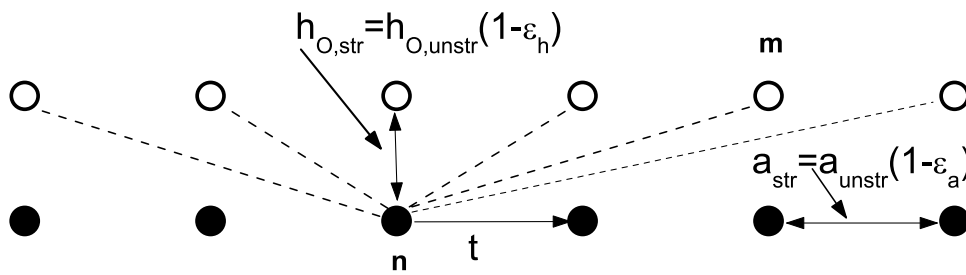


Fig. 1 The strained chain model lattice of cuprates. An electron performs hopping motion in a one-dimensional chain of the ions (lower chain — black circles) and interacts with all ions of an upper chain (open circles which is apical oxygen ions O(2)) via a density-displacement type force

$f_m(\mathbf{n})$ (dashed lines). The distance between the ions of lower chain a is set equal to CuO_2 in-plane lattice period of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$. The distance between the ions of lower chain and the ions of upper chain are assumed equal to h_o which is $\text{Cu}(1)\text{-O}(2)$ bond length of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$

Alexandrov and Kornilovitch in ref. [1] in order to mimic an interaction of a hole on CuO_2 plane with the vibrations of apical oxygen ions in the cuprates. Convincing evidence for a such coupling of in-plane holes with the c -axis polarized vibrations of apical oxygen ions comes from many experiments (for example [42]). Therefore, here we consider only that component of the electron-lattice force which represents an interaction of a hole on CuO_2 plane with the c -axis polarized apical oxygen vibrations. In addition, for the sake of simplicity, it is assumed that apical oxygen ions are dispersionless Einstein oscillators with the vibration frequency ω , and we estimate the mass renormalization factor g^2 within extended Holstein model (which is consistent with the ideality of Bose gas of intersite bipolarons). In that case, the mass renormalization factor g^2 for the given model lattice can be expressed as:

$$g^2 = \gamma \frac{E_p}{\hbar\omega}, \tag{2}$$

where

$$\gamma = 1 - \frac{\sum_{\mathbf{m}} f_{\mathbf{m}}(\mathbf{n}) f_{\mathbf{m}}(\mathbf{n} + \mathbf{a})}{\sum_{\mathbf{m}} f_{\mathbf{m}}^2(\mathbf{n})} \tag{3}$$

is a numerical coefficient,

$$E_p = \frac{1}{2M\omega^2} \sum_{\mathbf{m}} f_{\mathbf{m}}^2(\mathbf{n}) \tag{4}$$

is a polaron shift, M is apical oxygen ion’s mass and $f_{\mathbf{m}}(\mathbf{n})$ is the density-displacement type EPI force defined by analytical formula

$$f_{\mathbf{m}}(\mathbf{n}) = \frac{\kappa h_o (1 - \epsilon_h)}{[|\mathbf{n} - \mathbf{m}| (1 - \epsilon_a)]^2 + (h_o (1 - \epsilon_h))^2]^{3/2}}. \tag{5}$$

Here κ is some coefficient, $|\mathbf{n} - \mathbf{m}|$ is the distance measured in units of the lattice constant a , h_o is $\text{Cu}(1)\text{-O}(2)$ bond length, ϵ_a is the strain of the a -axis lattice period, and ϵ_h is the strain of h_o . The lattice strains are defined

as $\epsilon_a = (a_{unstr} - a_{str})/a_{unstr}$ and $\epsilon_h = (h_{o,unstr} - h_{o,str})/h_{o,unstr}$, where subscripts *unstr* and *str* stand for unstrained and strained, respectively. Thus, the positive (negative) value of the variable ϵ_i ($i = a, h$) corresponds to the compressive (tensile) strain. Equation (5) is a generalization of the force considered in ref. [1] (see Eq. (9) there). Such an explicit choice of the analytical formula for the force of EPI allows one to interrelate the temperature of Bose-Einstein condensation of the intersite bipolarons with the lattice strains through the mass of intersite bipolaron. The strains contribute to T_{BEC} not only through g^2 but also through bipolaron’s concentration n as upon deformation an initial volume V_0 of the sample changes and becomes $V(\epsilon_a, \epsilon_b, \epsilon_c) = V_0(1 - \epsilon_a)(1 - \epsilon_b)(1 - \epsilon_c)$. As a result, the concentration of intersite bipolarons becomes the function of the strains too:

$$n = n_0(1 + \epsilon_a)(1 + \epsilon_b)(1 + \epsilon_c). \tag{6}$$

In obtaining the last expression, we put $n_0 = N/V_0$ (N is the total number of intersite bipolarons in the sample) and neglected the terms of the quadratic order of smallness, i.e. $\sim \mathcal{O}(\epsilon^2)$. The above equations are the main analytical results of the model, according to which discussion of the experimental data for LSCO thin films will be done in the next section.

3 Results and Discussion

In the previous section, we expressed the temperature of Bose-Einstein condensation of intersite bipolarons T_{BEC} (Eq. (1)) through two basic parameters of a system: (i) the density of intersite bipolarons n and (ii) the exponent g^2 of the polaron mass enhancement. With the help of the above equations, one can study the dependence of the temperature of Bose-Einstein condensation T_{BEC} on the lattices strains ϵ_a (or ϵ_b) and ϵ_c through n and g^2 . The latter dependence, of course, originates from the polaronic effect. Here, we discuss

the possibility of application of Eq. (1) to LSCO films with a thickness of 500 Å grown on two types of substrates, namely, on LSAO and STO substrates. A common note to both cases (substrates) is that we consider the influence of the substrate to the superconducting properties of the thin film, in particular, to the value of T_c , only through the strains of the lattice constants of the thin films which are originated due to mismatch of lattice constants of the film and substrate. In our formulas, we use the numerical values of physical quantities in natural units, that is, in SI units, in order to easily compare the theoretically calculated results with the available experimental data. As in our study, the essential role is given to the electron-phonon interaction of CuO_2 in-plane charge carriers with the c-axis polarized vibrations of *apical* oxygen ions (i) we put $M=16$ a.m.u. ($2.6565032 \cdot 10^{-26}$ kg); (ii) for the *apical* oxygen ion's vibration frequency, we accept $\hbar\omega = 0.075$ eV ($1.2016324237 \cdot 10^{-20}$ J) which is common for all cuprates. And for the bipolaron concentration, we accept the value $n_0 = 1 \cdot 10^{21} \text{ cm}^{-3}$. Furthermore, we will associate the distance between the ions of lower chain a in Fig. 1 with the CuO_2 -plane lattice period of tetragonal $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$. And the distance between the ions of lower chain and the ions of upper chain h_O in Fig. 1 we will associate with the Cu(1)-O(2) bond length of tetragonal $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$. The distances a and h_O for the tetragonal $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ at different doping levels x (or Sr concentration) can be found in ref. [43]. As for the lattice constants of the LSCO thin films (LSAO and STO substrates), we took them from Fig. 13 and Table 3 of ref. [3]. Concerning the strain ϵ_a of the lattice constant a of LSCO thin films grown on LSAO and STO substrates, it is also given in Table 4 of the same ref. [3]. However, these values of the strains, according to our calculations, are more probably related to the state of the films and substrates at $T=295$ K, while superconductivity of LSCO cuprates occurs at relatively low temperatures of the order of 30 K. Then, it is natural to expect that the lattice strains at low temperatures will differ from those values of Table 4 of the same ref. [3]. Therefore, it would be more adequate to determine and use in our calculations the lattice strains of LSCO thin films corresponding to low temperatures of the order of 30 K. For that reason, we used the data of lattice periods from [43] corresponding to the temperature 10 K. Next, we calculated the numerical values of T_{BEC} of LSCO thin films grown on LSAO and STO substrates. In doing this, we firstly chose the value of polaron shift E_p in such a way that the calculated value of T_{BEC} in absence of the strains, i.e. $\epsilon_a=0$ and $\epsilon_h=0$, is equal to the experimental value of T_c of bulk LSCO. Secondly, since the value of ϵ_c is not given in Table 4 of ref. [3] in order to estimate the value of ϵ_c for 500 Å thick films, we used the existing correspondences between ϵ_a and ϵ_c of 2000 Å thick films of LSCO [9]. Thirdly, in calculating T_{BEC} at arbitrary ϵ_a and ϵ_h , for the strain ϵ_h , we accept a double value of the ϵ_c , i.e. $\epsilon_h = 2 \times \epsilon_c$, as according to

ref. [44] deformation of Cu(1)-O(2) bond length “*is roughly twice as large as the cell compression along the same direction (c-axis)*”. The calculated values of T_{BEC} of LSCO thin films, with different doping levels x , grown on LSAO and STO substrates are given in Table 1. These values of T_{BEC} are calculated for the doping levels $x=0.075, 0.1, 0.1125, 0.1250, 0.1375, 0.15, 0.2$ and 0.25 . For each doping level, the strains are calculated using the experimental lattice parameters of LSCO both bulk and film. The essential lattice parameters of LSCO both bulk and films are the lattice periods a and c of tetragonal LSCO as well as atomic position parameter $z[\text{O}(2)]$. The latter characterizes a position of O[2] *apical* oxygen with respect to CuO_2 plane. Using $z[\text{O}(2)]$ and c , one can easily determine the Cu[1]-O[2] distance by a formula $h_O = c \times z[\text{O}(2)]$. The numerical values of these data as well as the values of polaron shift E_p , polaron's mass m_p , in-plane polaron's mass m_{ab} and γ at different levels of Sr concentration x are summarized in the same Table 1. The mass of in-plane polaron m_{ab} is calculated by using the formulas $m_p = m_{ab}^{2/3} m_c^{1/3}$ and $\gamma_m = m_c/m_{ab}$. The latter is taken equal to 160 for LSCO at all doping levels [45]. In the same table, for the purpose of comparison, the experimental values of T_c of LSCO thin films are given too. From the table, one can see that there is a good agreement between calculated T_{BEC} of our model and experimental T_c of LSCO thin films grown on LSAO and STO substrates. In case of LSCO thin films grown on LSAO substrate, we performed calculations of T_{BEC} for two temperatures, namely, at $T=10$ K and $T=295$ K. While for LSCO thin films grown on STO substrate, we could not find measured lattice constants of the films in ref. [3] except the data for the film with doping level $x=0.15$. Therefore, for doping level $x=0.15$, we calculated T_{BEC} of LSCO thin films grown on STO films by using the data from Table 4 and Fig. 13 of ref. [3] while for other values of the doping levels we did the same calculations by using ϵ_a from Table 4 of ref. [3] and ϵ_c estimated from the experimental data of the lattice constants from ref. [43] for the temperature $T=10$ K. The theoretically obtained results are graphically presented in Fig. 2 too. The experimental values of the temperature of superconductivity T_c of LSCO bulk samples are taken from ref. [46] (dashed line). And the same for the films with the thickness of 500 Å grown on LSAO and STO substrates are taken from Fig. 16 of ref. [3]. As one can see from Table 1 as well as from Fig. 2, the theoretically calculated values of T_{BEC} are close to the experimental values of T_c of LSCO thin films. This agreement is satisfactorily in a whole region of the doping level. For the LSCO/LSAO system, at some values of the doping levels, namely at $x=0.1, 0.1125, 0.2$, we found a surprising match between T_{BEC} and T_c with the absolute accuracy of less than ± 1 K. In particular, we confirm an early obtained result of $T_c=39$ K for 500 Å thick $\text{La}_{1.9}\text{Sr}_{0.1}\text{CuO}_4$ film grown on LSAO substrate [3]. Meanwhile, for other values of doping levels of the LSCO/LSAO system,

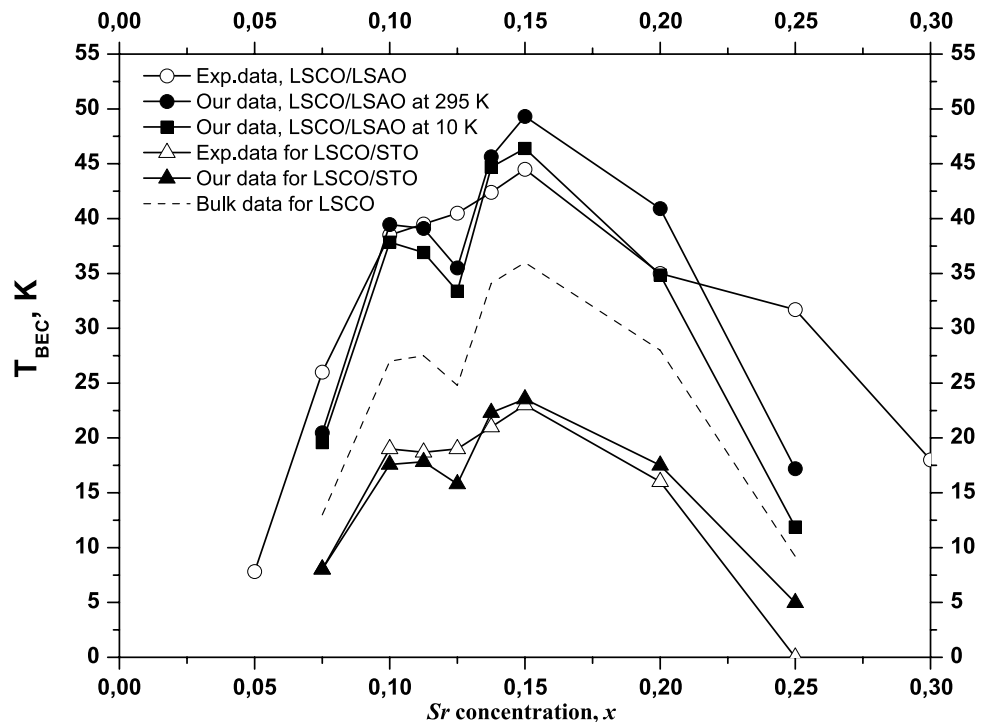
Table 1 The calculated values of T_{BEC} , E_p , m_p , m_{ab} and γ at different levels of Sr concentration x for $La_{2-x}Sr_xCuO_4$ thin films with a thickness of 500 Å grown on $LaSrAlO_4$ and $SrTiO_3$ substrates. The lattice parameters for bulk samples are taken from ref. [43], and the same for the films are taken from [3]. The strains along a -axis of the films as well as the experimental values of T_c of the films are also taken from [3]. The value of ϵ_c was estimated according to the existing correspondences between ϵ_a and ϵ_c of 2000 Å thick films of LSCO [9]

x		0.0750	0.1000	0.1125	0.1250	0.1375	0.1500	0.2000	0.2500
a , Å	Bulk LSCO	3.7861	3.7811	3.7785	3.7768	3.7750	3.7736	3.7640	3.7602
c , Å		13.1640	13.1700	13.1813	13.1859	13.1881	13.1973	13.2146	13.2214
$z[O(2)]$, Å		0.1835	0.1829	0.1829	0.1828	0.1827	0.1827	0.1819	0.1813
h_O , Å		2.4156	2.4088	2.4109	2.4104	2.4095	2.4111	2.4035	2.3970
a_{film} , Å	LSAO	3.7564	3.7564	3.7564	3.7564	3.7564	3.7564	3.7564	3.7564
	STO						3.7984		
c_{film} , Å	LSAO	13.2850	13.2900	13.2855	13.2890	13.2900	13.2950	13.2959	13.2952
	STO						13.1731		
ϵ_a , %	LSAO [3]	0.8750	0.7500	0.7230	0.6600	0.6150	0.5700	0.4400	0.3200
	STO [3]	-3.0600	-3.1900	-3.2350	-3.2800	-3.3250	-3.3700	-3.5100	-3.6300
ϵ_c , %	LSAO	-1.0259	-1.0300	-0.9525	-0.9531	-0.8309	-0.9273	-1.0766	-1.4346
	STO	0.7650	0.7975	0.8087	0.8200	0.8312	0.8425	0.8775	0.9075
E_p , eV	LSAO	0.4731	0.3991	0.4001	0.4105	0.3819	0.3740	0.3947	0.4916
	STO	0.5376	0.4549	0.4538	0.4660	0.4301	0.4246	0.4543	0.5825
γ	LSAO	0.6767	0.6784	0.6785	0.6788	0.6805	0.6789	0.6782	0.6757
	STO	0.7219	0.7239	0.7234	0.7237	0.7240	0.7237	0.7252	0.7273
m_{ab}, m_e	LSAO	13.1483	6.8073	6.8732	7.5627	5.8899	5.4407	6.5356	15.4496
	STO	32.5717	14.8700	14.6617	16.5292	11.7015	11.0831	14.8963	52.2740
m_p, m_e	LSAO	71.3800	36.9558	37.3137	41.0568	31.9756	29.5370	35.4808	83.8734
	STO	176.826	80.7268	79.5959	89.7343	63.5253	60.1682	80.8696	283.789
T_{BEC} , K	LSAO	20.4651	39.4593	39.1061	35.5103	45.6400	49.3165	40.9031	17.1950
	STO	8.0370	17.5829	17.8254	15.8049	22.3165	23.5520	17.5000	4.9800
T_c , K	LSAO [3]	26.0	39.0	39.5	40.5	42.4	44.5	35.0	31.7
	STO [3]	8.0	19.0	18.7	19.0	21.0	23.0	16.0	0

the absolute discrepancies of the calculated values of T_{BEC} from T_c are less than ± 5 K. The absolute discrepancies of the calculated values of T_{BEC} from T_c of LSCO/STO system are

less than ± 2.5 K. However, at some values of doping level x , the values of T_{BEC} differ from T_c significantly. This discrepancy, as is seen from Fig. 2, is more pronounced in the

Fig. 2 The phase diagram of LSCO films with a thickness of 500 Å in (T_{BEC}, x) plane. The experimental values of T_c of LSCO thin films grown on LSAO (STO) substrate are given by open circles (open triangles). For the LSCO/LSAO system, T_{BEC} is calculated for the temperatures 10 K (filled circles) and 295 K (filled squares). For the LSCO/STO system, T_{BEC} is calculated for the temperature 10 K (filled triangles). The dashed line presents the experimental values of T_c of bulk LSCO. The lines are a guide to the eye



overdoped regime. The reasons of the discrepancies we will discuss below.

Now, it would be useful to make general remarks on our model and the obtained results:

- (i) Our model takes into account the main features of cuprates, that is, the strong electron-phonon interaction, which determines the state and dynamics of charge carriers (polarons and bipolarons);
- (ii) Our model considers the cuprates as quasi-2D structure in which the dynamics of (bi)polarons is governed not only by the lattice dynamics of CuO_2 -plane (i.e. *ab*-plane) ions but also by the vibrations of the out of *ab*-plane ions which are *apical* oxygen ions;
- (iii) It is able to take also into account the lattice strains in the crystal structure of cuprates, in particular, the strains in the cuprate thin films which are subjected to the deformation in all direction simultaneously;
- (iv) As it is observed in many experiments our model gives high (low) value of T_{BEC} of thin film compared the bulk value of T_{BEC} when *ab*-plane of the cuprate film is compressed (stretched). The same is true when *c*-axis of the cuprate film is stretched (compressed);

In turn, we have to in some way interpret the discrepancies between our T_{BEC} and experimental T_c at certain values of doping levels. There might be several reasons of the discrepancies. They are:

- (i) The use of the extended Holstein-Hubbard (or Fröhlich-Coulomb) model at strong coupling regime and nonadiabatic limit while in a real situation the cuprates might be in some doping regimes at moderate values of electron-phonon coupling as well as in intermediate regimes of adiabaticity;
- (ii) The choice of model lattice which is the simplest one. It is one-dimensional. In reality, one should consider the three-dimensional crystal structure of LSCO;
- (iii) The choice of electron-phonon “density-displacement” type force in the form of Eq. (5) that might lead to the underestimation the value of E_p in the cuprates like the case with Fröhlich type EPI [47];
- (iv) The estimation the mass of polaron (bipolaron) within the extended Holstein model thus ignoring the correlation effects that is important in the cuprates;
- (v) And the last one is the use of assumption that bipolarons form an ideal gas (their Bose-Einstein condensation temperature is determined by the Eq. (1)). As it is seen from our results, Fig. 2, such the assumption may be valid in overdoped and optimally doped regimes, but in the overdoped regime it underestimates the values of T_{BEC} ;

All the above points might contribute to the full discrepancy. Apart from the above theoretical reasons, there might be the reasons from the experimental sites that measure T_c by various methods. In the literature, one finds the experimental works in which T_c reported (measured) as onset temperature, midpoint temperature and the temperature at which the resistivity becomes 90% of the value at the onset temperature as well as the zero-resistivity temperature. In our opinion, these circumstances might also cause some inconsistency between our T_{BEC} and experimental T_c . Nevertheless, as one can see from our numerical results, in general, our model satisfactorily explains the value of T_c of LSCO thin films grown on LSAO and STO substrates. Then, one could conclude that even with such a type of simple assumptions our model captures the essential physics of the LSCO.

It is remarkable that T_{BEC} versus x dependence obtained in our model has a dome-like shape similar to the shape of T_c versus x dependence of bulk LSCO, i.e. the phase diagram of bulk LSCO. In such circumstances, Fig. 2 can be interpreted as the phase diagram of the strained LSCO thin films. It is interesting that the phase diagram of LSCO thin films exhibits a feature, near doping level $x=1/8$, similar to the observed “1/8”-anomaly in the phase diagram of bulk LSCO. Of course, this “1/8”-anomaly (feature) of the phase diagram of LSCO thin films is originated from *polaronic-structural* effect. And it is one of the conclusions of our model that gives realistic phase diagram for the strained LSCO thin films in (T_c, x) plane with “1/8”-anomaly feature.

4 Conclusion

We studied the thin films of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ cuprate within the framework of the extended Holstein-Hubbard (or Fröhlich-Coulomb) model. Namely, we were interested with the values of T_c of LSCO thin films grown on LSAO and STO substrates. We accepted the bipolaronic mechanism of superconductivity for cuprates in which T_c is associated with the Bose-Einstein condensation temperature T_{BEC} of the ideal gas of the intersite bipolarons. In our model, T_{BEC} we defined from Eq. (1) where both mass of (bi)polaron and concentration of bipolarons depend on the crystal lattice structure through the lattice constants and lattice period's strains. In turn, the all lattice parameters (periods and strains) of bulk LSCO depend on doping level. In addition, the lattice parameters of the films depend on the type of substrate. Eventually, we were able to interrelate T_{BEC} through the lattice parameters of the films. Then, we calculated the values of Bose-Einstein condensation temperature T_{BEC} of the ideal gas of intersite bipolarons in LSCO thin film grown on LSAO and STO substrates. In doing this, we take into account the real values of lattice constants of the thin films and strains. The calculated

values of Bose-Einstein condensation temperature T_{BEC} of the ideal gas of intersite bipolarons in LSCO thin film grown on LSAO and STO substrates are in satisfactory agreement with the values of the temperature of superconductivity T_c of the considering thin films. Some discrepancies between our T_{BEC} and experimental T_c might be the result of several reasons. We discussed the reasons of the discrepancies too. T_{BEC} versus x dependence obtained in our model has a dome-like shape similar to the shape of T_c versus x dependence of bulk LSCO. This dependence has the “1/8”-anomaly feature and can be interpreted as a phase diagram of strained LSCO thin films.

Declarations

Conflict of Interest The authors declare no competing interests.

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