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ОГЛАВЛЕНИЕ

On correlation of T_c and Cu-O$_{apex}$ distance in single layered cuprates

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Annotation. Superconductivity of the single-layered cuprates 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 single-layered cuprates, a relation between the temperature of Bose-Einstein condensation (T_{BEC}) of an ideal gas of the intersite bipolarons and the lattice parameters is established. While doing that (relation), the chain model of cuprates, proposed by Alexandrov and Kornilovitch in ref.[1], is used. It is shown that the calculated values of the temperature of Bose-Einstein condensation of the bipolarons in the single-layered cuprates correlate with (in direct ratio to) the distance between planar Cu and *apical* oxygen O(2) of the single-layered cuprates. Using reasonable experimental values of the lattice parameters of single-layered cuprates we found both quantitative and qualitative agreement between T_{BEC} and T_c of the studying systems.

Key words: single-layered cuprates, superconductivity, Bose-Einstein condensation, bipolaron, critical temperature.

I. Introduction. Copper-oxide (cuprate) high-temperature superconductors (HTSC) can currently be divided into several families: La-, Y-, Bi-, Tl- and Hg-based cuprates. Although cuprates differ in composition, their crystal structures share similarities and, moreover, common structural units. These are copper-oxygen (CuO_2) planes, CuO_6 octahedrons and charge reservoirs. It is believed that charge reservoirs serve as suppliers of charge carries (hole or electron) and superconducting properties of the cuptates mainly determined by the dynamics of charge carriers near CuO_2 planes. It was also established that superconducting properties of the cuprates strongly depend on the positions of the ions that are out of CuO_2 plane. Experiments show that nearest ion to CuO_2 plane which is *apex* oxygen has profound effect on the superconducting properties of the cuprates [2]. Namely, it turns out that the critical temperature of superconductivity T_c of the cuprates is directly proportional to the distance from the in-plane Cu ion to the apex O(2) ion, h_O i.e. the longer the h_O, the higher T_c. The latter effect is more pronounced in single layered cuprates like $La_{2-x}Sr_xCuO_4$, $Bi_2Sr_2CuO_{6+\delta}$, $Tl_2Ba_2CuO_6$ and $HgBa_2CuO_4$ with the T_c equal to 36 K, 40 K, 85 K and 90 K, respectively. There are a few works in the literature that discuss the issue within the different models [3, 4, 5, 6, 7]. A valuable conclusion of Sakakibata et al., is the importance to keep higher the distance between the apical oxygen and in-plane copper atoms h_O, and to decrease the in-plane Cu-O bond lengths.

Though, the above theoretical works (models) give some ideas on and discuss why the value of T_c differs from one cuprate to another one cannot say that the models are able to take into account all and/or essential features of the phenomenon under consideration. The main features of the cuprates are their quasi two dimensional crystal structure and presence of the strong electron-phonon interaction (EPI). Indeed, it is well understood that EPI plays an important role in the cuprates [8, 9], in particular, EPI that involves *apical* oxygen atoms determines dynamics of charge carrier in copper-oxygen (CuO_2) plane [10]. And EPI is strong enough to favour (bi)polaron formation [11]. The strong EPI manifests itself as polaronic nature of charge carriers in the cuprates [12]. The results of many experiments on normal and superconducting state of the cuprates are also in satisfactory agreement with a (bi)polaronic approach to cuprate superconductivity [13, 14, 15]. One may conclude that the above theoretical models consider the cuprates totally ignoring the strong EPI, and consequently ignoring the possibility of polaron and/or bipolaron formation. They ignore, in particular, the interaction of in-plane (CuO_2) charge carriers with the c- polarized vibrations of the apex oxygen atoms. The existence of correlation between the position of apex oxygen and the value of T_c was established in early period of study of cuprates [16]. The experimental data obtained so far and tested models for different cuprates suggest that the phenomenon of high-T_c superconductivity is complex and differ for various compounds. Nevertheless, there are common features, too. As a consequence, at present, one experiences a need of a model that able to explain all experimental data, in particular, the differences among the values of T_c, from universal points of view.

In present paper, we will try to fill this blank and introduce relation between T_c with lattice parameters of cuprate that will be in both qualitative and quantitative agreement with the experiments. While 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 consequently their Bose-Einstein condensation (BEC) giving rise to the superconductivity. Thus, here we associate T_c with the Bose-Einstein condensation temperature, T_{BEC} , of intersite bipolarons. Consideration of the issue within the framework of bipolaronic model of superconductivity is useful because of the experimental evidences that the superconducting state of cuprates "*cannot be described by the standard BCS theory, anywhere in the phase diagram*" [17]. The main idea of our approach was given in the works [18, 19, 20, 21]. In the work [18], the values of T_c of $La_{1.85}Sr_{0.15}CuO_4$ and $La_{1.9}Sr_{0.1}CuO_4$ thin films, which were grown on LSAO and STO substrates, were satisfactorily explained. The work [19] extends our approach to $RBa_2Cu_3O_{7-\delta}$ cuprates. The recent works [20, 21] are devoted to the explanation of doping dependencies of T_c of $La_{2-x}Sr_xCuO_4$ thin films and the uniaxial pressure (strain) derivatives of T_c of $La_{2-x}Sr_xCuO_4$ bulk samples.

II. Theoretical model. According to the bipolaron model of superconductivity, HTSC cuprates are due to the Bose-Einstein condensation of a gas (or liquid) of the intersite bipolarons [22]. Accepting simple assumptions such as: (i) the intersite bipolarons form an ideal gas; (ii) mass of bipolaron is twice of polaron's mass i.e. $m_{bp} = 2m_p$ and that the cuprates are (iii) in strong EPI limit and (iv) on nonadiabatic regime, one can estimate the Bose-Einstein condensation temperature, T_{BEC}, of the ideal gas of the intersite bipolarons [18, 19]

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

where $\hbar$ (k_B) is Planck's (Boltzmann's) constant, m^* is the bare band mass (is set equal to mass of free electron), n is density of the intersite bipolarons and g^2 is the mass renormalization factor of polaronic system. The above reasonings can be justified by the facts that (i) concentration of charge carriers in the cuprates is relatively small (dilute limit); (ii) the Coulomb repulsion between bipolarons is significantly reduced in the cuprate oxides by the ionic screening (page 132 of Ref. [23]). The mass renormalization factor g^2 is defined as [1]

$$g^2 = \gamma \frac{E_p}{\hbar\omega}, \quad (2)$$

where

$$\gamma = 1 - \frac{\sum_m f_m(n) f_m(n+a)}{\sum_m f_m^2(n)} \quad (3)$$

is a numerical coefficient,

$$E_p = \frac{1}{2M\omega^2} \sum_m f_m^2(n) \quad (4)$$

is a polaron shift, M is *apical* oxygen ion's mass and $f_m(n)$ is the *density-displacement* type EPI force defined by analytical formula

$$f_m(n) = \frac{\kappa h_O}{[|(n-m)|^2 + h_O^2]^{3/2}}. \quad (5)$$

Here κ is some coefficient, $|n-m|$ is the distance measured in units of the lattice constant a, h_O is Cu(1)-O(2) bond length. For numerical results we rely on the model lattice of chain model of cuprates (Fig. 1) and calculate g^2 for that lattice. In the chain model of cuprates an electron (hole) performs hopping motion in an one-dimensional chain of Cu(1) ions (a chain of black circles) and interacts with all apex oxygen O(2) ions via a density-displacement type force $f_m(n)$. The distance between the copper Cu(1) ions of the lower chain a is set equal to CuO_2 in-plane lattice period of cuprates. The distance between the planar Cu(1) ion and the apical O(2) ion is assumed equal to h_O which is Cu(1)-O(2) bond length of cuprates.

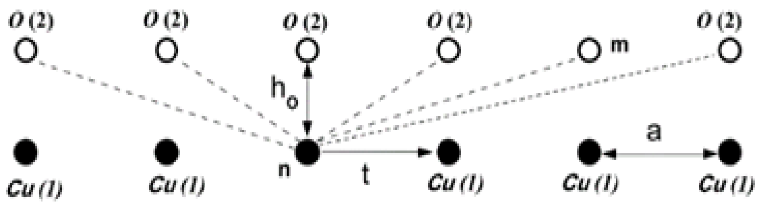

Figure 1. *Chain model of cuprates.*

The *density-displacement* type force Eq. (5) was introduced by 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 [24]). 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 and for the sake of simplicity, we assume that *apical* oxygen ions are dispersionless Einstein oscillators with the vibration frequency ω. In addition, we estimate the mass renormalization factor g^2 within extended Holstein model (which is consistent with the ideality of Bose gas of intersite bipolarons).

The above equations are the main analytical results of the model, according to which we study the dependence of T_c on the lattice parameters of single layered cuprates in the next section.

III. Results and discussion. In the previous section, we expressed T_{BEC} of intersite bipolarons (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 T_{BEC} on the lattices parameters a and h_O. 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· 10^{-26} kg); (ii) and for the bipolaron concentration, we accept the value $n_0 = 1 \cdot 10^{21}$ cm $^{-3}$ which is common for all cuprates. Furthermore, we will associate the distance between the ions of lower chain a in Fig.1 with the CuO_2-plane lattice period a of tetragonal phase of cuprates. 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 cuprate.

A starting point of our numerical analysis is setting up a values of E_p =0.4 eV and *apical* oxygen ion's vibration frequency $\hbar\omega$=0.075 eV (1.2016324237· 10^{-20} J) for $La_{1.85}Sr_{0.15}CuO_4$ single-layered cuprate. The latter choices provide a coincidence of our T_{BEC}, calculated using the lattice parameters of $La_{1.85}Sr_{0.15}CuO_4$, with the experimental value of T_c =36 K of the above cuprate.

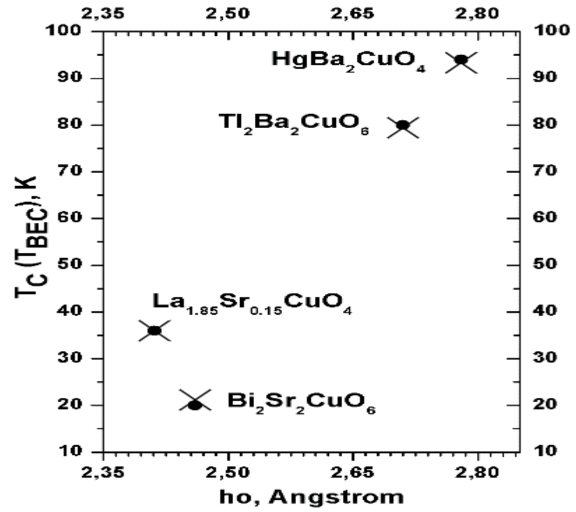

Figure 2. *The values of experimental T_c (filled black circles •) and theoretically calculated T_{BEC} (×) versus h_O for single-layered cuprates.*

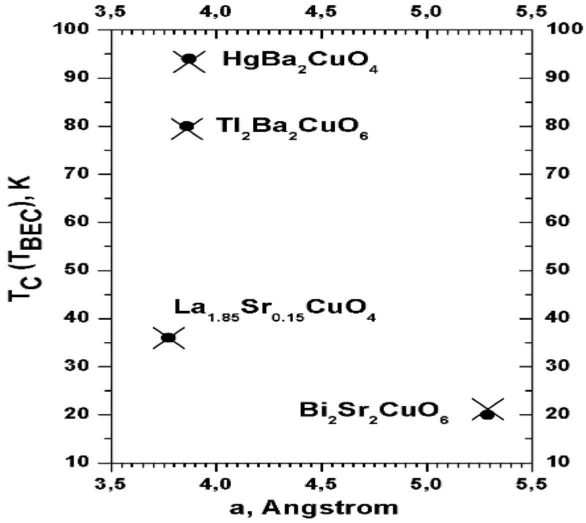

Figure 3. *The values of experimental T_c (filled black circles •) and theoretically calculated T_{BEC} (×) versus lattice period a for single-layered cuprates.*

Then, we proceed with the calculation of T_{BEC} for other single-layered cuprates using the well-known experimental values of their lattice periods (can be found in Refs.[25, 26]). Our T_{BEC} are in satisfactorily agreement with the experimental values of T_c of single-layered cuprates when one uses the certain values of *apical* oxygen ion's vibration frequency.

Namely, we put $\hbar\omega$ equal to 80 meV, 58 meV and 55 meV in our calculations for $Bi_2Sr_2CuO_{6+\delta}$, $Tl_2Ba_2CuO_6$ and $HgBa_2CuO_4$ single-layered cuprates, respectively. These values of *apical* oxygen ion's vibration frequency lie in the range of the experimentally found frequencies between 40 meV and 75 meV [27]. The calculated values of T_{BEC} for considering cuprates are are given in Fig.2 and Fig.3. In the same Fig.2 and Fig.3 the experimental values of T_c of silgle-layered $La_{1.85}Sr_{0.15}CuO_4$, $Bi_2Sr_2CuO_{6+\delta}$, $Tl_2Ba_2CuO_6$ and $HgBa_2CuO_4$ cuprates are presented for a purpose of comparison. As one can see from Fig.2 and Fig.3 the theoretically calculated values of T_{BEC} are close to the experimental values of T_c of single-layered cuprates. Furthermore, in agreement with the experimental observations, in our model the high value of T_{BEC} corresponds to the longer Cu-O$_{apex}$ distance (Fig.2) and the shorter in-plane lattice period (Cu-O distance) (Fig.3).

A note should be done on the value of T_{BEC} (and T_c) of $Bi_2Sr_2CuO_{6+\delta}$ which is smaller than that of $La_{1.85}Sr_{0.15}CuO_4$ despite the fact that the former has longer h_O distance than the latter. This case can also be explained within our model. The fact is that $Bi_2Sr_2CuO_{6+\delta}$ compound has a larger lattice period along the copper-oxygen plane than $La_{1.85}Sr_{0.15}CuO_4$ compound. The relative absolute value of the difference between the copper-oxygen in-plane lattice periods of the compounds as great as 43% while that for h_O is relatively small, 2%. CuO_2-plane of $Bi_2Sr_2CuO_{6+\delta}$ is severely expanded compared to the CuO_2-plane of $La_{1.85}Sr_{0.15}CuO_4$. Our calculations clearly show that with such an arrangement of lattice ions, the value of T_{BEC} (and T_c) decreases despite the fact that the lengthening of the Cu-O$_{apex}$ distance slightly increases T_{BEC} (and T_c).

IV. Conclusion. We considered the single-layered $La_{1.85}Sr_{0.15}CuO_4$, $Bi_2Sr_2CuO_{6+\delta}$, $Tl_2Ba_2CuO_6$ and $HgBa_2CuO_4$ cuprates within the framework of the extended Holstein-Hubbard (or Fröhlich-Coulomb) model. Namely, we were interested with the values of T_c of the above cuprates. 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. So, T_{BEC} depends on the lattice parameters of the cuprate. Then, we calculated the values of Bose-Einstein condensation temperature T_{BEC} of the ideal gas of intersite bipolarons in the studying cuprates. While doing this, we take into account the real values of lattice constants of the single-layered cuprates. The calculated values of Bose-Einstein condensation temperature T_{BEC} of the ideal gas of intersite bipolarons are in satisfactory agreement with the values of the temperature of superconductivity T_c of the considering cuprates. Our approach presented here can be applied to other cuprates, too.

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