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STRAIN (PRESSURE) STUDY OF $RBa_2Cu_3O_{7-\delta}$ CUPRATE: A BIPOLARON APPROACH

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Abstract: The extended Holstein model (EHM) was introduced in Ref [1], primarily for the explanation of smallness of charge carrier's mass in the cuprates. The lattice of Figure 1A was introduced by Alexandrov and Kornilovitch in Ref. [1] in order to mimic the interaction of a hole on the CuO_2 plane with the vibrations of *apical* ions in the cuprates (Figure 1B is considered in Ref. [6]). Such one-dimensional lattices have similarity with some ion's arrangements in the real structure of RBa2Cu3$O_{7-\delta}$ cuprates. Indeed in the both lattices the upper chain (open circles) represents apical ions of oxygen at position *O(4)*.

Keywords. bipolaron, strain (pressure), Bose-Einstein condensation, cuprates

Introduction

The extended Holstein model (EHM) was introduced in Ref [1], primarily for the explanation of smallness of charge carrier's mass in the cuprates. Quite recently, one of us (B.Ya.Ya.) extended an application of the EHM to La-based cuprate films under pressure (strained films) [2]. Namely, in that work, a unified approach for studying the influence of pressure (stress or strain) on the temperature of Bose-Einstein condensation of intersite bipolarons was proposed. Uniaxial strain derivatives of Bose-Einstein condensation temperature (T_{BEC}) of intersite bipolarons were calculated. Having accepted the bipolaronic scenario as a ground for high-T_c superconductivity of cuprates, the experimental results on the influence of lattice mismatch to the critical temperature (T_c) of La-based high-T_c films were explained. In particular, the results of two experiments [3,4] were explained within the framework of the EHM and the bipolaronic theory of superconductivity. The main features of the model proposed in Ref. [2] are: (i) compressive pressure (strain) in the *ab*-plane of cuprates enhances T_{BEC} and (ii) compressive pressure (strain) along *c*-axis of cuprates reduces T_{BEC}. Such variations of the T_c of cuprates with respect to applied pressure (strain) are often observed [5]. The proposed model allows one to interrelate strains in each axis with each other and to study their cumulative effect on T_{BEC}.

Here, we continue to study the influence of strain induced by external pressure or lattice mismatch on T_{BEC} for different lattices. Special attention will be given to the possibility of qualitative explanation of such phenomena as sign difference of the strain (pressure) derivatives of T_c of $RBa_2Cu_3O_{7-\delta}$ cuprates (R stands for Yb, Y, Dy or Gd) along the *a*- and *b*-axes. $RBa_2Cu_3O_{7-\delta}$ compounds stand apart from other cuprates (with the CuO_2 planes only) because of the presence of *Cu-O* chains along the *b*-axis in the crystal structure. Strong anisotropy of crystal structure gives rise to the anisotropy of electronic, thermodynamic, transport and other properties of the $RBa_2Cu_3O_{7-\delta}$ family of materials. In particular, uniaxial strain derivatives of the critical temperature, T_c, along crystallographic axes *a* and *b* have opposite sign: $\partial T_c/\partial \varepsilon_a < 0$ and $\partial T_c/\partial \varepsilon_b > 0$. The value of the uniaxial strain derivative of the critical temperature of cuprates along *c*-axis, $\partial T_c/\partial \varepsilon_c$, lies in a wide range, but all values are negative. Therefore, at present, development of a model that explains the uniaxial strain (pressure) derivatives of T_c from the universal point of view and takes into account strong electron-phonon interaction in the cuprates is one of the most important research tasks in the way of our understanding the microscopic origin of high-T_c phenomena. Our model, proposed in [2], does not suffer from the above-mentioned imperfections.

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Below we show that the EHM and Bose-Einstein condensation scenario of intersite bipolarons, if one accepts the latter to be responsible for high-T_c superconductivity of cuprates, are able to qualitatively explain the sign difference of $\partial T_c/\partial \varepsilon_a < 0$ and $\partial T_c/\partial \varepsilon_b > 0$.

2. The Model Hamiltonian and lattices

The lattice of Figure 1A was introduced by Alexandrov and Kornilovitch in Ref. [1] in order to mimic the interaction of a hole on the CuO_2 plane with the vibrations of *apical* ions in the cuprates (Figure 1B is considered in Ref. [6]). Such one-dimensional lattices have similarity with some ion's arrangements in the real structure of $RBa2Cu3O_{7-\delta}$ cuprates. Indeed in the both lattices the upper chain (open circles) represents apical ions of oxygen at position *O(4)*. The lower chain of Fig.1A consists of copper Cu(1) ions of Cu(1)-O(1) chain or copper Cu(2) ions of CuO_2 plane. Fig.1B resembles arrangement of oxygen O(2) ions of CuO_2 plane and O(4) oxygen ions. The occurrence of an anisotropy of charge carrier's mass in $RBa_2Cu_3O_{7-\delta}$ compounds we model here by the orientational dependence of the "density-displacement" type electron-phonon interaction on the relative positions of out of plane ions with respect to copper-oxygen (CuO_2) plane. The latter effect is caused by the anisotropy of the structure $RBa_2Cu_3O_{7-\delta}$ of compounds. In this way we can model an interaction of the hole belonging to copper-oxygen plane with the apical oxygen ions at O(4) positions. Though such a primitive model lattices far from the real structure of $RBa_2Cu_3O_{7-\delta}$ compounds, we will see below that they are able to capture the essential physics of the influence of strain (pressure) to T_c of $RBa_2Cu_3O_{7-\delta}$ compounds. It has been shown that within the EHM intersite bipolarons tunnel in the first order of polaron tunneling and mass of the intersite bipolaron has the same order as polaron's mass [7]. For the sake of simplicity, we suppose here that intersite bipolarons form an ideal gas of charge carriers and mass of bipolaron is $m_{bp} = 2m_p$ (this point does not lead to loss of generality). Then the temperature of Bose-Einstein condensation of the intersite bipolarons is defined as

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

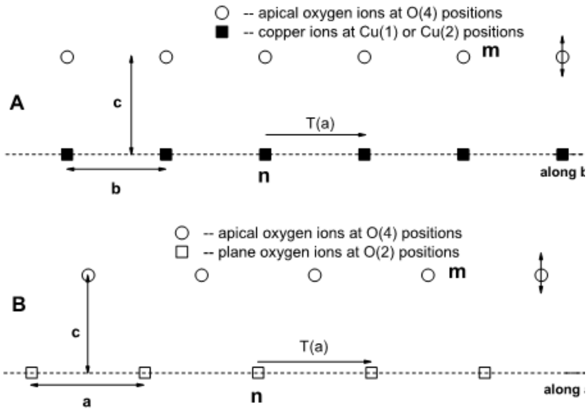

Figure 1: An electron hops on a lower chain of ions (squares) and interacts with the *c*-polarized vibrations of ions (open circles) of an upper chain, via a density-displacement type of force $f_m(\boldsymbol{n})$. The distances between the chains ($|\boldsymbol{c}|$) and between the ions ($|\boldsymbol{a}|$ or $|\boldsymbol{b}|$) of the same chain are assumed equal to 1.

Here k_B is Boltzmann constant and n is density of intersite bipolarons. For the ideal gas of charge carriers one can estimate polaron's mass within EHM. In the strong electron-phonon coupling limit and nonadiabatic regime estimation of the polaron's renormalized mass yields $m_p/m^* = \exp[g^2]$ [1] (see also [8]), where

$$g^2 = \frac{1}{2M\hbar\omega^3} \sum_m [f_m^2(\boldsymbol{n}) - f_m(\boldsymbol{n}) f_m(\boldsymbol{n}+\boldsymbol{a})]. \quad (2)$$

and $m^* = \hbar^2/2T(a)a^2$ is the bare band mass. In order to consider the stress of a lattice and its influence on the (bi)polaron mass, and consequently on the temperature of Bose-Einstein condensation of intersite bipolarons, the analytical expression

$$f_m(\boldsymbol{n}) = \frac{\kappa c(1-\varepsilon_c)}{[|(\boldsymbol{n}-\boldsymbol{m})(1-\varepsilon_i)|^2 + (\boldsymbol{c}(1-\varepsilon_c))^2]^{3/2}} \quad (3)$$

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will be used for the density-displacement type force ($i = a$ or b). Here κ is some coefficient, and ε_a, ε_b and ε_c are lattice strains along the a-, b- and c-axes, respectively. The distance $|\boldsymbol{n}-\boldsymbol{m}|$ is measured in units of the lattice constant $|\boldsymbol{a}| = 1$ (or $|\boldsymbol{b}| = 1|$). The lattice strains are defined as $\varepsilon_a = (a_{unst} - a_{str})/a_{unst}$, $\varepsilon_b = (b_{unstr} - b_{str})/b_{unst}$ and $\varepsilon_c = (c_{unst} - c_{str})/c_{unst}$, where subscripts *unstr* and *str* stand for unstrained and strained, respectively. Eq. (3) is a generalization of the force considered in Ref. [1] (see Eq.(9) therein) and allows one to interrelate the temperature of Bose-Einstein condensation of the intersite bipolarons with the lattice strains through the mass of the intersite bipolaron.

3. Results and discussion

The expression Eq. (1) expresses T_{BEC} 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. Eq.(1) allows one to study the dependence of T_{BEC} on the model lattices (Fig.1) strains ε_a, ε_b or ε_c at constant *n*. This dependence, of course, originates from polaronic effects. We have calculated the values of T_{BEC} as a function of the strains along the *b*-axis ε_b and *c*-axis ε_c for the model lattice given in Fig.1A. The results are given in Fig.2. Here we put $n = 1 \cdot 10^{21} sm^{-3}$ and $\kappa^2/2M\hbar\omega^3 = 5.885$ in order to coincide T_{BEC} in the absence of the strains with the bulk value of $T_c \approx 91$ K of *YBCO* cuprates. The results of calculation of T_{BEC} for the lattice in Fig.1B are shown in Fig.3. As one can see from Fig.2, compressive strain along *b*-axis gives rise to increase the value of T_{BEC}, while that along *c*-axis acts on the contrary. Compressive strain along both the *a*-and *c*-axes in the model lattice of Fig.1B lowers the value of T_{BEC}. The uniaxial strain derivatives of T_{BEC} for the model lattice given in Fig.1A at $\kappa^2/2M\hbar\omega^3 = 5.885$ are: $\partial T_{BEC}/\partial\varepsilon_b \approx +278\,K$ and $\partial T_{BEC}/\partial\varepsilon_b \approx -1210\,K$. The same uniaxial strain derivatives of T_{BEC} for the model lattice given in Fig.1B at $\kappa^2/2M\hbar\omega^3 = 9.265$ are: $\partial T_{BEC}/\partial\varepsilon_a \approx -115\,K$ and $\partial T_{BEC}/\partial\varepsilon_c \approx +874\,K$.

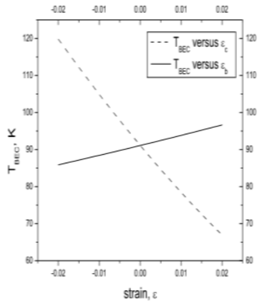
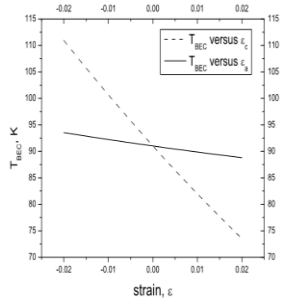


Figure 2. The temperature of Bose-Einstein condensation of the intersite bipolarons as a function of strains along the *b*-axis ε_b (solid line) and along the *c*-axis ε_c (dashed line) for the lattice of Fig.1A. Here we put $\kappa^2/2M\hbar\omega^3 = 5.885$ in order to coincide T_{BEC} at $\varepsilon_i = 0$ $(i = b, c)$ with the bulk value of $T_c \approx 91$ K of *YBCO* high-T_c cuprates at optimal doping.



Fifure 3. The temperature of Bose-Einstein condensation of the intersite bipolarons as a function of strains along *b*-axis ε_a (solid line) and along *c*-axis ε_c (dashed line) for the lattice of Fig.1B. Here we put $\kappa^2/2M\hbar\omega^3 = 9.265$ in order to coincide T_{BEC} at $\varepsilon_i = 0$ $(i = a, c)$ with the bulk value of $T_c \approx 91$ K of *YBCO* high-T_c cuprates at optimal doping.

The obtained results clearly demonstrate a strong dependence of T_{BEC} on the arrangement of ions in the lattice. This has a crucial effect on the value of T_{BEC}. The sign of $\partial T_{BEC}/\partial\varepsilon$ is different for *a*- and *b*-axes, which is caused by mutual arrangements of ions. In particular, for the lattices in Fig.1A and Fig.1B one finds $\partial T_{BEC}/\partial\varepsilon_b \approx +278\,K$ and $\partial T_{BEC}/\partial\varepsilon_a \approx -115\,K$, respectively. The uniaxial strain derivatives, $\partial T_{BEC}/\partial\varepsilon_c$ of the two lattices are both negative. These results clearly show that the two model lattices in some ways qualitatively characterize the situations in $RBa_2Cu_3O_{7-\delta}$ compounds under pressure (strain). Thus, compressive pressure (or strain) along the *b*-axis (*a*-axis) increases (*lowers*) the value of T_{BEC} in analogy with increase (decrease) of T_c of $RBa_2Cu_3O_{7-\delta}$ compounds

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under compressive pressure (or strain) in the same direction. The effect of compressive pressure (strain) along the *c*-axis is similar to that of along the *a*-axis. In terms of quantity, one should be aware that our findings obtained relative to the lattices in Fig.1, and not to real cuprates. Considering more real model structures similar to the real structure of *YBCO* cuprates, one may obtain better value of $\partial T_{BEC}/\partial \varepsilon_i$, close to the $\partial T_C/\partial \varepsilon_i$ of *YBCO*. On the other hand, the values of the uniaxial pressure (strain) derivative of T_c along crystallographic axes $i = a, b, c,$ measured, in different experiments, are spread over a wide range, and in some cases contradicts to each other. Welp et al. were the first to present direct measurements of $\partial T_C/\partial p_i$ for the untwinned $YBa_2Cu_3O_{7-\delta}$ single crystal [9]. Their results are: $\partial T_C/\partial p_a = -2.0 \pm 0.2K/GPa$, $\partial T_C/\partial p_b = +1.9 \pm 0.2K/GPa$ and $\partial T_C/\partial p_c = -0.3 \pm 0.1K/GPa$. Bud'ko et al. obtained uniaxial pressure (strain) derivatives of the critical temperature of $RBa_2Cu_3O_{7-\delta}$ cuprate from the hydrostatic pressure dependence, measured on the films of different crystalline orientations [10]. According to Ref. [10], $\partial T_C/\partial p_a = -3.06 \pm 0.35K/GPa$ ($\partial T_C/\partial \varepsilon_a \approx -3.62 \pm 50K$), $\partial T_C/\partial p_b = +0.38 \pm 0.18K/GPa$ ($\partial T_C/\partial \varepsilon_b \approx -301 \pm 30K$)and $\partial T_C/\partial p_c = +3.45 \pm 0.43K/GPa$ ($\partial T_C/\partial \varepsilon_c \approx +239 \pm 24K$). Pickett, in his paper [11], quoting to the experimental results of Refs. [9,12], gives unexpected data: $\partial T_C/\partial \varepsilon_a \approx +212\,K$, $\partial T_C/\partial \varepsilon_b \approx -244\,K$ and $\partial T_C/\partial \varepsilon_c \approx -8\,K$. One can see that our results are close to the $\partial T_C/\partial \varepsilon_i$ of Ref. [10].

Now let's imagine that one has a hypothetic a quasi-two-dimensional anisotropic lattice in which the interaction of charge carriers (holes or electrons) with out-of-plane ions is strong, and that when external pressure is applied along the *a*- (*b*-) axis this interaction occurs in the analogous way to that as in the one-dimensional lattice of Fig.1B (Fig.1A). Then, the quasi-two-dimensional anisotropic lattice has all features of *YBCO* cuprates with respect to the influence of uniaxial strain (pressure) on T_c. Indeed, solving the system of equations

$$\sum_j C_{ij}\frac{\partial T_{BEC}}{\partial p_j} = \frac{\partial T_{BEC}}{\partial \varepsilon_i}, \quad (10)$$

with the set of elastic constants of the *YBCO* cuprate (all in GPa) $C_{aa} = 231$, $C_{ab} = 132$, $C_{ac} = 71$, $C_{bb} = 268$, $C_{bc} = 95$ and $C_{cc} = 186$ taken from Ref. [13], one finds $\partial T_{BEC}/\partial p_a = -0.65$), $\partial T_{BEC}/\partial p_b = +3.58$) and $\partial T_{BEC}/\partial p_{ca} - 6.27$ (all in K/GPa). Use of other set of elastic parameters (all in GPa) $C_{aa} = 283$, $C_{ab} = 148$, $C_{ac} = 83.1$, $C_{bb} = 304$, $C_{bc} = 109$ and $C_{cc} = 236$ taken from Ref. [14], yields $\partial T_{BEC}/\partial p_a = -0.54$, $\partial T_{BEC}/\partial p_b = +2.91$ and $\partial T_{BEC}/\partial p_{ca} - 4.86$ (all in K/GPa). These findings indicate that the Bose-Einstein condensation scenario of the ideal Bose-gas of intersite bipolarons is, *in principle*, able to qualitatively explain the uniaxial strain (pressure) experiments, regarding the effect of the strain (pressure) on T_c of *YBCO* cuprates. Quantitative discrepancies of our results and experimental data may be the result of several factors: (i) the simplicity of the model lattices under consideration. In reality one should consider more complex structures than in Fig.1; (ii) the choice of the analytical formula for the density-displacement type electron-lattice force; (iii) the assumption that intersite bipolarons form an ideal Bose-gas: in reality, due to other factors, there may be deviation from the ideal case, leading to the formation of a nonideal Bose-gas or Bose-liquid; (iv) superconductivity of the *YBCO* cuprate may be due not only to electron-phonon interaction, but may also have contributions from other interactions as well. These factors suggest that we should undertake more comprehensive research on the studied problem.

The proposed model serves as a universal tool for studying strain (pressure) induced effects in the cuprates. Its common features are relevant to all cuprates. In contrast with some theoretical approaches the model allows one to interpret the influence of pressure (strain) on T_{BEC} (T_c) along each axe, independently of the others. Meanwhile, the model is able to account for interference of strains between axes via the Poisson relation $\nu = \varepsilon_a/\varepsilon_c$ or $\nu = \varepsilon_b/\varepsilon_c$. This may be also useful in theoretical studies of cuprate films grown on different substrates.

4. Conclusion

In conclusion, we have studied the effect of uniaxial strain (pressure) on the temperature of Bose-Einstein condensation of intersite bipolarons within the framework of the Extended Holstein model. Uniaxial strain derivatives of T_{BEC} are determined for different lattices. It is found that $\partial T_{BEC}/\partial \varepsilon_i$ depends strongly on the arrangement of ions in the lattice. In particular, it may be positive or negative. The results for the lattices under study (Fig.1) in some way mimic the influence of uniaxial strain (pressure) on the critical temperature, T_c, of YBCO cuprates. The calculated values of the pressure derivatives of $T_{\rm BEC}$ for the hypothetic lattice qualitatively agree with the observed values of $\partial T_{BEC}/\partial p_i$ (i=*a*, *b*, *c*) for *YBCO* cuprates.

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