Theoretical Study on the Pressure Induced T_c Change in $YBa_2Cu_3O_x$

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Pressure effect on the critical temperature, T_c, of the $YBa_2Cu_3O_x$ superconductor was considered in the frame of a simple theoretical model which as a starting point assumes that T_c vs. pressure, P, dependence can be described by an inverted parabola. Available experimental results on T_c behavior under pressure were analyzed as a function of the zero pressure hole concentration in the superconducting CuO_2 planes, $n_h(P = 0\ \text{GPa}) = n_{h0}$, for different constant values of P. Maximum T_c that can be achieved under pressure was estimated and discussed in relation to the $n_{h0} = 1/8$ doping and establishment of charge and spin order. The results obtained here were used to estimate increase of the hole concentration in the CuO_2 planes which occurs as a result of pressure induced oxygen reordering.

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1. Introduction

Experimentally established fact that pressure application leads to the enhancement of the critical transition temperature T_c in $YBa_2Cu_3O_x$ class of high-T_c superconductors, points out to the possibility of the synthesis of materials with ambient pressure T_c higher than the current record of 138 K held by the thallium doped mercury cuprate of $(Hg_{0.8}Tl_{0.2})Ba_2Ca_2Cu_3O_{8.33}$ composition [1].

Investigations on how pressure affects superconducting behavior may also help in elucidating microscopic mechanism of superconductivity, which despite many years of intense research efforts, both theoretical and experimental, still remains beyond our comprehension. Many high pressure experiments conducted thus far on the $YBa_2Cu_3O_x$ system revealed that pressure application changes both structural and electronic properties of the material thus leading to the change of the superconducting behavior [2–11].

Since the critical temperature T_c is the complex function of many different parameters, it is generally very difficult to incorporate into a theory all the relevant factors and establish appropriate model which would correctly describe all the peculiarities of the T_c behavior under pressure. In $YBa_2Cu_3O_x$ the pressure effect, $\mathrm{d}T_c/\mathrm{d}P$, significantly changes with change of oxygen concentration, x, and it also strongly depends on the temperature at which the high pressure experiment is conducted [3, 9]. At temperatures higher than 240 K pressure triggers oxygen diffusion in the oxygen deficient CuO_x planes which results in the formation of longer CuO chains with increased ability to provide additional holes for the superconducting CuO_2 planes. Therefore the pressure effect is much more pronounced at temperatures above 240 K which is especially evident in the case of oxygen poor samples where short chains prevail, while in the almost completely oxygenated samples this effect is almost negligible since all oxygen atoms are already incorporated into very long CuO chains.

At low temperatures the oxygen atoms are frozen in the lattice and the pressure application cannot provoke their movements. In $YBa_2Cu_3O_x$ system size of the pressure effect is also greatly influenced by the directional axes of pressure application, so that it can even become negative when the pressure is applied along the b crystallographic axes (the one along which the CuO chains are aligned) [12].

Having in mind all these aspects of such a complex behavior of $YBa_2Cu_3O_x$ superconductor under pressure, it is not hard to understand why the pressure experiments tending to reveal microscopic mechanism of high-T_c superconductivity are usually conducted on those members of the cuprate family superconductors whose structure does not include chain planes.

Nevertheless, the $YBa_2Cu_3O_x$ superconductor and its behavior under pressure still remain subject of interest of many experimental and theoretical research groups. Till date several theoretical studies have been conducted on the pressure effect in cuprate superconductors [13–20]. The simplest way to attack this problem is to employ the modified pressure induced charge transfer (PICT) model which involves charge transfer from the CuO_x to the CuO_2 planes, as well as intrinsic contribution which originates from the pressure induced structural changes and from all the other changes in the system caused by pressure not involving the charge transfer [9, 14].

In this paper we will also employ a simple phenomenological PICT type model to investigate the pressure effect on $YBa_2Cu_3O_x$. We will consider how the critical temperature T_c changes with pressure depending on the initial (zero pressure) hole concentration in the CuO_2 planes.

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2. Theoretical model

We start from the well known empirical relation between the critical temperature T_c and the hole concentration n_h in the CuO_2 planes, which is valid in the case of $YBa_2Cu_3O_x$ compound as well as for many other high-T_c superconductors [21]:

$$T_c(n_h) \cong T_c^{max} \times \left[1 - A \times (n_{h0} - n_{h,opt})^2\right], \quad (1)$$

where $A = 1/(n_{h,opt} - n_{h,min})^2$, $n_{h,opt}$ is the optimal hole concentration at which T_c reaches the maximum value T_c^{max}, and $n_{h,min}$ is the minimum concentration of holes in the CuO_2 planes below which superconductivity vanishes. The maximum T_c, T_c^{max}, depends on the particular system and for $YBa_2Cu_3O_x$ compound $T_c^{max} = 93$ K, while the optimum hole concentration, $n_{h,opt}$, is equal to 0.16 in many cuprate superconductors as for $YBa_2Cu_3O_x$ as well [21]. Samples with $n_{h0} < n_{h,opt}$ are usually termed as underdoped and those with $n_{h0} > n_{h,opt}$ as overdoped. In Eq. (1) all parameters, T_c^{max}, A, and $n_{h,opt}$, may be functions of pressure describing different structural and electronic structure changes that pressure application may induce.

It is well confirmed by the Hall effect measurements that pressure application causes hole transfer from the chain planes to the CuO_2 planes [9, 10]. Therefore it is not surprising that the T_c vs. pressure dependence, measured for the constant value of oxygen concentration x, can be, similarly to $T_c(n_h)$ dependence, described by an inverted parabola [21]:

$$T_c(P) \cong T_c^{max*} \times \left[1 - B \times (P - P_{opt})^2\right]. \quad (2)$$

In the above relation T_c^{max*} is the maximum T_c which can be achieved in the sample with some constant oxygen concentration x. Therefore T_c^{max*}, as well as the parameters B and P_{opt} are some functions of x, but since samples with the same x can have different zero pressure T_c's and hole concentrations (depending on the oxygen order in the CuO_x planes established during the sample preparation) we will assume these parameters to be functions of n_{h0}. Generally T_c dependence on P and n_{h0} can be expressed through a single equation of the type

$$T_c(n_{h0}, P) \cong T_c^{max}(P) \times \left[1 - \beta(P) \times (n_{h,0} - n_{h0,opt}(P))^2\right]. \quad (3)$$

In the above equation T_c dependence on P is expressed through the pressure dependence of the parameters T_c^{max}, β, and $n_{h0,opt}$. In this work we will try to establish how these parameters depend on pressure and to determine what is the maximum T_c that can be achieved under pressure in $YBa_2Cu_3O_x$ superconductor.

3. Discussion of the obtained results and conclusions

One of the most thorough experimental investigation on the superconducting properties of the $YBa_2Cu_3O_x$ system under pressure was conducted by Sadewasser and his coworkers [5] on the five samples with different zero pressure critical temperatures, and therefore with different zero pressure hole concentrations. In Fig. 1 we present experimental results for T_c vs. P dependences extracted from Ref. [5] (represented by points), and at the same figure we show the results obtained from the fit to Eq. (2) (the fit curves are represented by solid lines). One can observe that the experimental results fit the relation (2) reasonably well. Thus we obtained parameters of Eq. (2) for five samples with different $n_{h,0}$ which enabled calculation of T_c's for a wider range of pressures.

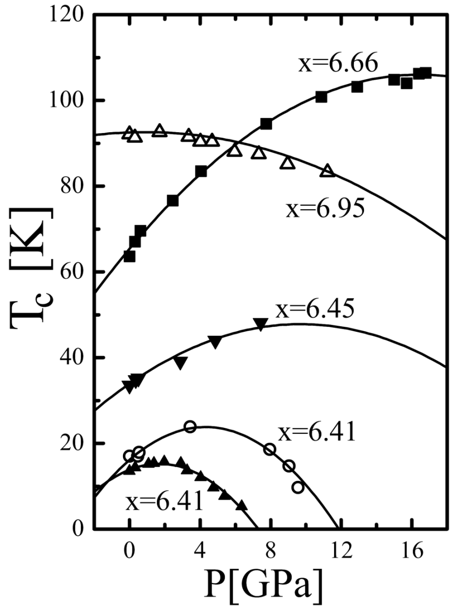

Fig. 1. T_c dependence on pressure P, for different values of oxygen concentration x. Experimental data points are extracted from Ref. [5], and the solid lines are fits to Eq. (2).

Further, we have analyzed behavior of T_c as a function of zero pressure hole concentration, n_{h0}, at different constant values of pressure. We found that T_c as a function of n_{h0}, is described very well by Eq. (3) for all values of pressure considered.

In order to illustrate how the $T_c(n_{h0})$ dependence behaves under pressure we presented in Fig. 2 $T_c(n_{h0})$ dependence for $P = 0$ GPa, together with $T_c(n_{h0})$ parabola obtained for $P = 4$ GPa. One can observe that under pressure the whole $T_c(n_{h0})$ parabola became somewhat narrower and that it was moved to the left, towards lower n_{h0} values. Also, the maximum T_c was significantly increased and it was achieved in the sample with lower zero pressure hole concentration. The similar behavior was established for a large set of different values of pressure P, and therefore we were able to determine parameters $T_c^{max}(P)$, $\beta(P)$, and $n_{h0,opt}(P)$ of Eq. (3).

Behavior of these parameters with pressure is shown in Fig. 3. Since the T_c^{max} vs. P dependence displays a parabolic like behavior it can be fitted to the equation

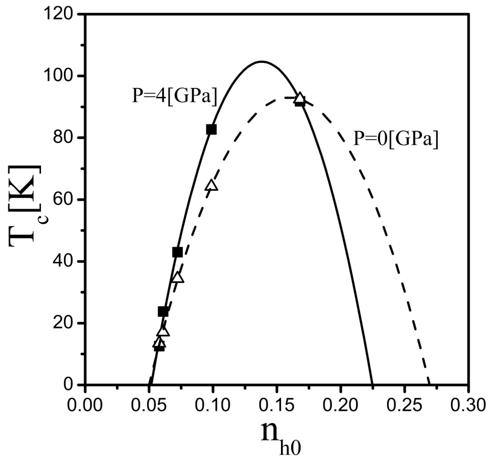

Fig. 2. T_c vs. n_{h0} dependence for $P = 0$ GPa and for $P = 4$ GPa. Solid lines are parabolic fits to the experimental results from Ref. [5] which are represented by points.

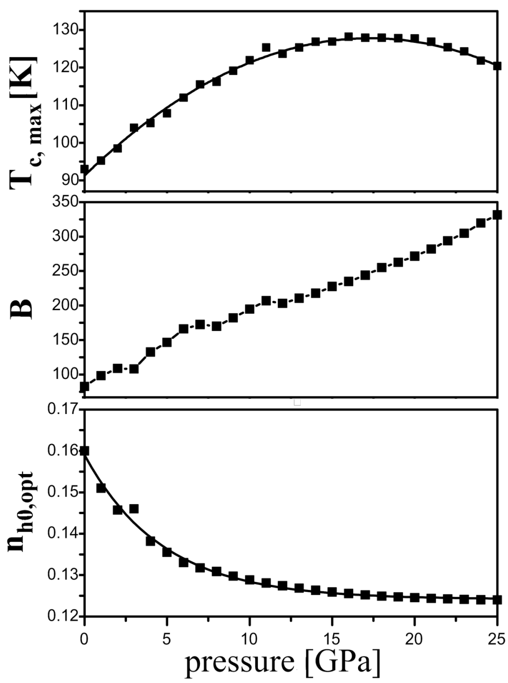

Fig. 3. Coefficients T_c^{max}, B and $n_{h0,opt}$ as a function of pressure P. In part (a) and (c) of the figure solid lines represent fits to the parabolic and exponential dependence, respectively, while in the part (b) solid line is a linear fit.

of the type (2). Thus we obtained that maximum T_c attainable under pressure in $YBa_2Cu_3O_x$ superconductor is approximately 128 K, and it can be reached for $P_{opt} \approx 17$ GPa. This result is in agreement with our previous estimation [22] ($T_c^{max} \approx 131$ K, $P_{opt} \approx 18$ GPa) obtained by the use of the similar model. However, to our knowledge there is no experimental evidence on what is the maximum T_c in the $YBa_2Cu_3O_x$ compound under pressure.

Dependence of the B parameter on the pressure is shown in the part (b) of Fig. 3. It can be seen that parameter B almost linearly increases with pressure in the range from ambient pressure up to the 25 GPa. Since the parameter B actually measures width of $T_c(n_{h0})$ parabola at its base, its increase with pressure indicates that $T_c(n_{h0})$ parabola is narrowing which we already observed in Fig. 2. Though we obtained that the parameter B increases with pressure in the whole range of pressures considered here, we expect that it will reach its maximum for some higher value of pressure.

In part (c) of Fig. 3 we show how the parameter $n_{h0,opt}$ changes with pressure. One can observe that $n_{h0,opt}$ decays exponentially with pressure saturating at $n_{h0,opt} \approx 0.124$ for very high pressures ($P > 20$ GPa).

It is interesting to note that the maximum T_c under pressure can be achieved in the sample with $n_{h0} \approx 0.125$ value which is the one corresponding to establishment of the charge and spin order (stripe phase) which is known to compete with superconductivity (the so called "1/8 anomaly"). Though the static stripes were not found in $YBa_2Cu_3O_x$ superconductor under normal conditions, it is believed that this "1/8 anomaly" is a generic feature to all cuprate superconductors [23].

Recently the charge density wave (CDW) order was experimentally found in the ortho-II phase of the $YBa_2Cu_3O_x$ [24, 25] and this CDW order is also expected to be the most stabilized at $n_{h0} \approx 0.125$. The fact that the model presented predicts maximum T_c under pressure to be reached in the sample with this specific n_{h0} value complies with some previous observations that pressure application may cause depinning of the stripes thus giving an extra boost to superconductivity [26]. Suppression of the charge ordering by pressure was experimentally confirmed in some superconductors [27] and these results may indicate that the same pressure induced charge ordering suppression mechanism might be also going on in $YBa_2Cu_3O_x$ system.

Until this point we have considered experimental findings on the $T_c(P)$ behavior when the pressure is applied at temperatures low enough to prevent oxygen reordering in the oxygen deficient CuO_x planes. However if the pressure is applied at higher temperatures it will enable movements of oxygen atoms and their ordering into longer CuO chains which are known to be better hole dopants than the short ones (only CuO chains longer than 3 or 4 oxygen atoms can transfer holes) [28, 29]. This will inevitably have consequences on T_c behavior with pressure.

Experimental results from Ref. [5] on the behavior of $T_c(P)$ curve when the oxygen reordering is involved are shown in the inset of Fig. 4, together with $T_c(P)$ curve obtained when no oxygen diffusion is present for the sample with $x = 6.41$ and $n_{h0} = 0.0606$. Since the simple charge transfer model presented does not enable calculation of hole concentration increase with pressure, we

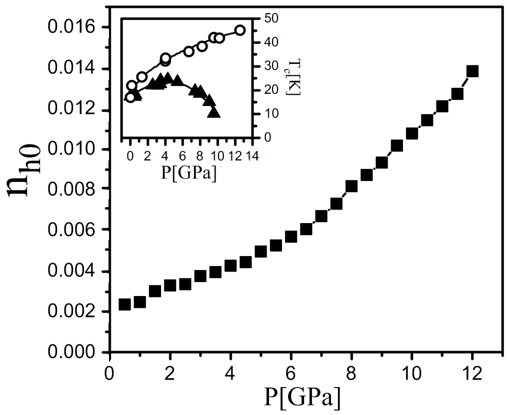

Fig. 4. Change of the hole concentration produced by the pressure induced oxygen reordering at different pressures evaluated at zero pressure. In the inset there are shown experimental results for T_c vs. P dependences for $x = 6.41$ sample, with pressure applied at two different temperatures. The experimental points are extracted from Ref. [5] and the solid lines are guides to the eye.

will determine concentration of additional holes provided to the CuO_2 planes due to the pressure induced oxygen ordering. Employing Eq. (3) and the known values of the parameters T_c^{max}, β, and $n_{h0,opt}$ as well as the results on T_c's under pressure measured at 298 K and below 200 K, we were able to calculate the difference $\Delta n_{h0}(P) = n_{h0}^{298K}(P) - n_{h0}^{200K}$. Note that while n_{h0}^{200K} is the hole concentration in the sample calculated at zero pressure, n_{h0}^{298K} is the hole concentration that the sample would have at zero pressure but possessing the oxygen arrangement in the chain planes achieved by the action of pressure P.

In Fig. 4 we plot difference $\Delta n_{h0}(P)$ as a function of pressure up to the $P = 12$ GPa. One can observe that in the considered range of pressures $\Delta n_{h0}(P)$ continually increases, reaching the 0.014 value for $P = 12$ GPa, which means that initial hole concentration is increased for approximately 23%. This implies that the oxygen order in the chain planes is significantly improved under pressure applied at high enough temperature. Though $\Delta n_{h0}(P)$ increases in the whole range of pressures presented further pressure increase will inevitably lead to the saturation of the hole concentration generated by the pressure induced oxygen ordering, once the maximum possible oxygen order under given conditions (determined by the temperature, pressure and oxygen concentration x) is reached.

In summary we have analyzed available experimental data on $T_c(P)$ dependence in the high-T_c $YBa_2Cu_3O_x$ superconductor by using a simple phenomenological model which assumes that $T_c(P)$ dependences measured for samples with different constant oxygen concentrations x, can be described by an inverted parabola. It was established that for different constant values of pressure, critical temperature T_c as a function of zero pressure hole concentration can be, to a good approximation, described by a parabolic type dependence. Maximum T_c that can be achieved under pressure in $YBa_2Cu_3O_x$ is found to be 128 K and it can be reached at $P \approx 17$ GPa in the sample with $n_{h0} \approx 0.125$. This particular value of the hole concentration is also the one for which the charge ordering, which is known to suppress superconductivity, is at its strongest. Therefore, one can conclude that application of pressure enhances superconductivity through deterioration of the charge ordering phase [26]. Additionally we have also considered how the pressure affects the oxygen order in the chain planes and we found that the oxygen ordering is significantly improved under pressure.

Acknowledgments

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