Pressure Dependence of T_c in Y-Ba-Cu-O Superconductors

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By considering the recent widely accepted dispersion of electronic structure in cuprates, we analyze the pressure effect on the superconducting transition temperature T_c in Y-Ba-Cu-O systems. Two intrinsic variables, i.e., the effective attractive interaction V_{eff} and the hole concentration n_H in the CuO_2 plane, are proposed to be responsible for the pressure effect on T_c. Theoretical calculations agree well with experiments. Our results also suggested that the in-plane lattice parameter dependence of effective attraction V_{eff} obeys $d\ln V_{\text{eff}}/d\ln a = -4 \sim -2$ for Y-Ba-Cu-O systems.

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The pressure dependence of the transition temperature T_c of copper oxide high-T_c superconductors (HTSCs) is of fundamental interest for elucidating the microscopic mechanism of the superconducting state as well as for finding new materials with higher critical temperature by using the chemical pressure [1,2]. The initial study of $La_{2-x}Ba_xCuO_4$ under pressure triggered the discovery of the first compound with T_c higher than liquid nitrogen temperature, $YBa_2Cu_3O_7$ [3], proving that investigations under pressure can provide knowledge for searching for new material with higher T_c. Very recently, Locquet *et al.* [4] reported a doubling T_c of 49.1 K in the $La_{1.9}Sr_{0.1}CuO_4$ films grown on the $SrLaAlO_4$ substrate by tuning epitaxial strain. This demonstrates strongly that a higher T_c can be realized for a cuprate at ambient pressure under the application of chemical pressure.

Although the pairing mechanism responsible for the high-T_c superconductivity continues to remain elusive, it is generally believed that one of the key parameters controlling the T_c values is the charge carrier concentration n_H in the CuO_2 planes. It has been postulated that the application of high pressure leads to the change of n_H within the unit cell resulting in the pressure dependence of T_c, which was supported by a number of measurements [1,2,5,6]. However, attempts at a quantitative analysis of the dependence of T_c on pressure, based solely on this pressure-induced charge transfer mechanism, have not been particularly successful, suggesting that additional variables might be important [7–11]. There is evidence that the buckling angle of CuO_2 planes in the high-T_c cuprates is also important in attaining superconductivity with a distinct value of T_c. It has been found that increasing pressure causes the buckling angle to decrease [12,13]. Detailed experiments revealed that T_c increases with the buckling angle decreasing and tends to a constant when the buckling angle remains zero [14]. Very recently, Chmaissem *et al.* [15] found a clear scaling between T_c and the buckling angle of the CuO_2 planes. It is therefore indicated clearly that the buckling angle of the CuO_2 planes should be related directly with the effective pairing interaction leading to high-T_c superconductivity in HTSCs. That is, the intrinsic variables that would best describe the pressure dependence of T_c are just the variables that are used in the description of T_c itself. Transition temperature T_c is mainly influenced by two factors. One is the carrier concentration of the CuO_2 plane. The other one is the effective pairing interaction leading to superconductivity, although its microscopic interaction mechanism is still unknown at present.

In this Letter, we address this issue by studying hole-doped superconductors $YBa_2Cu_3O_{7-\delta}$ and $YBa_2Cu_4O_8$. A theoretical model is presented for pressure effect on T_c in the hole-doped HTSCs based on a widely accepted dispersion of electronic structure and the general relation between T_c and hole concentration. The oxygen content dependence of dT_c/dP in $YBa_2Cu_3O_{7-\delta}$ and the variations of T_c with pressure are predicted for $YBa_2Cu_3O_7$ and $YBa_2Cu_4O_8$. Our results compare well with experiments.

It is now well known that the superconducting transition temperature T_c in the cuprates varies approximately in an inverted parabolic manner with the hole concentration of the CuO_2 planes [16]. This behavior can be obtained by solving the BCS equation with $d_{x^2-y^2}$-wave order parameter $\Delta_k = \Delta_0 f_k$, $f_k = (\cos k_x - \cos k_y)/2$, and a phenomenological dispersion relation for holes in the CuO_2 plane, as evidenced from the angle-resolved photoemission studies [17,18],

$$\varepsilon_k = 0.166\,25\cos k_x \cos k_y + 0.046(\cos 2k_x + \cos 2k_y), \tag{1}$$

$$1 = \frac{V_{\text{eff}}}{2N}\sum_k f_k^2 \frac{1}{\varepsilon_k - \mu}\tanh\left(\frac{\varepsilon_k - \mu}{2T_c}\right), \tag{2}$$

along with the constraint condition for the hole concentration n_H:

$$n_H = \frac{1}{2} - \frac{1}{2N}\sum_k \tanh\left(\frac{\varepsilon_k - \mu}{2T_c}\right), \tag{3}$$

where V_{eff} is an effective pairing interaction which is directly related to the mechanism responsible for the

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high-T_c superconductivity. μ is the chemical potential and N the number of sites. It is worth emphasizing that the sum in the k space is taken over the entire Brillouin zone.

Considering the two intrinsic pressure variables, $n_H(P)$ and $V_{\rm eff}(P)$, one can use Eqs. (2) and (3) to study the pressure effect. Our starting point is that the pressure dependence of T_c is simply a function of these two intrinsic variables,

$$T_c(P) = T_c[n_H(P), V_{\rm eff}(P)]. \tag{4}$$

This hypothesis is similar to that studied by others [10,11]. It should be noted that the necessity of using two independent variables has been previously recognized by several groups in describing the pressure dependence of T_c, e.g., the pressure-induced charge transfer (PICT) models [7–9]. In the PICT models, the maximum value of the transition temperature at optimal doping ($T_c^{\rm max}$) is usually assumed to be another pressure sensitive variable besides the hole concentration n_H. However, its implications for investigating the pressure dependence of T_c have not been clarified yet. Since one must have the knowledge of dT_c/dP before using the PICT models; it is difficult to predict either the value of dn_H/dP or the value of $dT_c^{\rm max}/dP$ at optimal doping within the PICT models; most quantities should be determined experimentally. While in the present approach, most quantities can be calculated theoretically once the underline effective pairing interaction $V_{\rm eff}$ is known. There are more physical reasonings for taking $V_{\rm eff}(P)$ instead of $T_c^{\rm max}$ as an intrinsic variable: (1) for conventional superconductors, one only needs to know $V_{\rm eff}$ to determine T_c and associate physical properties. To use $V_{\rm eff}$ preserves historical as well as theoretical continuity. (2) $V_{\rm eff}$ is the driving force for superconductivity. It represents directly the underline physical process, while $T_c^{\rm max}$ is just the outcome of $V_{\rm eff}$.

To the first order in P, we have $n_H(P) = n_H + (dn_H/dP)P$ and $V_{\rm eff}(P) = V_{\rm eff}[1 + (d\ln V_{\rm eff}/dP)P]$. The initial pressure derivative of T_c is then calculated from Eqs. (2) and (3) as

$$\frac{dT_c}{dP} = \left(\frac{2T_c^3}{NI}\sum_k f_k^2 Q_k - \frac{T_c^2}{NI}\sum_k f_k^2 \frac{W_k}{\varepsilon_k - \mu}\right)\frac{dn_H}{dP} + \left(\frac{T_c^2}{NIV_{\rm eff}}\sum_k W_k\right)\frac{d\ln V_{\rm eff}}{dP}, \tag{5}$$

with

$$I = 2T_c\left(\frac{1}{2N}\sum_k(\varepsilon_k - \mu)W_k\right)\left(\frac{1}{2N}\sum_k f_k^2 Q_k\right) - \left(\frac{1}{2N}\sum_k(\varepsilon_k - \mu)W_k\right)\left(\frac{1}{2N}\sum_k f_k^2\frac{W_k}{\varepsilon_k - \mu}\right) + \left(\frac{1}{2N}\sum_k W_k\right)\left(\frac{1}{2N}\sum_k f_k^2 W_k\right),$$

where $W_k = \mathrm{sech}^2[(\varepsilon_k - \mu)/2T_c]$ and $Q_k = (\varepsilon_k - \mu)^{-2}\tanh[(\varepsilon_k - \mu)/2T_c]$. From Eqs. (4) and (5), one notices that in order to study the pressure dependence of $T_c(P)$ and dT_c/dP, one must have a knowledge of the values of dn_H/dP and $d\ln V_{\rm eff}/dP$. The pressure-induced change of n_H can be obtained from the bond-valence-sum analysis [19]. In the study of pressure effect of the conventional superconductors, Gladstone, Jensen, and Schrieffer [20] found that the pressure dependence of the electron-phonon coupling strength K ($= N_0 V_{\text{el-ph}}$) for the transition metals obeys $d\ln K/d\ln v = +2.5 \pm 0.7$, where v is the volume of the superconductor. There is not much information on the change of the effective attractive interaction $V_{\rm eff}$ with pressure in the high-T_c cuprates so far. Whether the effective attraction $V_{\rm eff}$ originated from the electron-electron interaction or electron-phonon interaction, one can always assume that $V_{\rm eff}$ varies with the in-plane lattice parameter along the a axis direction as $a^{-1}\exp(-\beta a)$, regardless what underline microscopic pairing mechanism is. In general, β is material dependent. Thus we have the pressure-induced relative change of $V_{\rm eff}$ as $d\ln V_{\rm eff}/dP = (1 + \beta a)\kappa_a$, where $\kappa_a = -d\ln a/dP$ being the lattice compressibility along the a axis.

Based on the structural data for $YBa_2Cu_3O_{7-\delta}$ compounds determined by neutron diffraction [21], one can evaluate the pressure-induced change of n_H, dn_H/dP, in the framework of bond-valence-sum analysis. The Cu-O(i) bond compressibility can be estimated by using the anisotropic bond model [22]. In the $YBa_2Cu_3O_x$ system, the superconductivity occurs for a $n_H^{\rm min} \sim 0.0$ and the maximum T_c is attained at a value of $n_H^{\rm opt} \sim 0.25$ holes [7,16]. The corresponding Cu valences, $V_{\rm Cu}^{\rm min} = 2.082$ and $V_{\rm Cu}^{\rm opt} = 2.135$, are obtained from the bond-valence-sum analysis [19], respectively. Following Jorgensen *et al.* [23], we obtained a value of $dn_H/dP = 8.08 \times 10^{-3}$ holes/GPa for $YBa_2Cu_3O_{6.93}$. This value is in the range of 6.5×10^{-3} and 1.1×10^{-2} holes/GPa in $YBa_2Cu_3O_{7-\delta}$ ($\delta \approx 0$) determined by other groups [6,8,23]. dn_H/dP was found to decrease with increasing oxygen content x. The value of dn_H/dP in the fully oxygenated $YBa_2Cu_3O_7$ should be smaller than that in $YBa_2Cu_3O_{6.93}$. It is reasonable to take $dn_H/dP = 8.0 \times 10^{-3}$ holes/GPa for $YBa_2Cu_3O_7$ in the following calculations.

Calculation of $T_c(P)$ was carried out for the fully oxygenated $YBa_2Cu_3O_7$ compound with $T_c = 93.5$ K [24], which is near the optimum hole concentration but slightly overdoped. Following Almasan *et al.* [7], we took $T_c^{\rm max} = 94$ K for the optimally doped $YBa_2Cu_3O_{7-\delta}$ compound, which yields $V_{\rm eff} = 0.1571$ eV from Eqs. (1)–(3). With the above determined parameters along with the lattice compressibility $\kappa_a = 2.22 \times 10^{-3}$ GPa^{-1} [23], from Eqs. (1)–(4) we can calculate the variation of T_c with pressure once having a knowledge of the coefficient βa. Results are displayed in Fig. 1. We found that experimental data points of Refs. [24,25] roughly lie on our theoretical curves. The maximum T_c on the $T_c \sim P$ curve is exhibited at $P \sim 1.6$, 4.0, and 6.2 GPa for $\beta a = 1$,

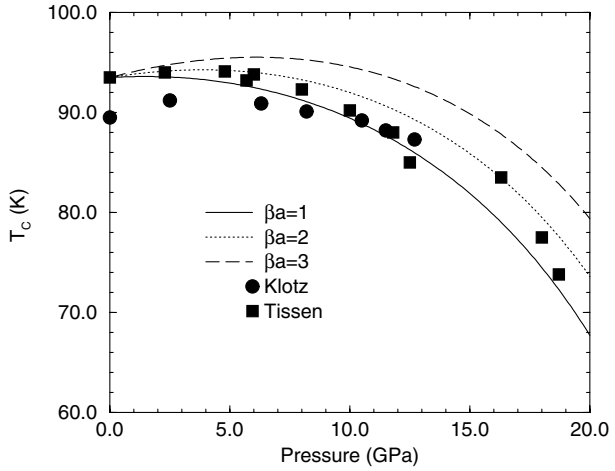

FIG. 1. Calculated values of T_c with pressure P in the fully oxygenated $YBa_2Cu_3O_7$ compound with $T_c = 93.5$ K up to 20 GPa.

2, and 3, respectively. The experimental points of Tissen *et al.* [24] distribute well on the $T_c \sim P$ curves. It is therefore indicated that the pressure dependence of the effective interaction V_{eff} obeys $d\ln V_{\text{eff}}/dP = (2 \sim 4)\kappa_a$ in $YBa_2Cu_3O_7$.

The oxygen content dependence of dT_c/dP of $YBa_2Cu_3O_x$ can be obtained according to Eq. (5) with reasonable coefficient βa. The lattice compressibilities κ_a are determined from the anisotropic bond model [22] by using the crystal structural data of Jorgensen *et al.* [21] The theoretical results along with the experimental data [7,26–28] are shown in Fig. 2. The calculated dT_c/dP exhibits positive value over a large doping range and decreases monotonically with increasing x. Qualitatively, theoretical data are consistent with experiments although there does not exist a plateau of 4.3 K/GPa for $6.4 \leq x \leq 6.8$ as those reported by Almasan *et al.* [7],

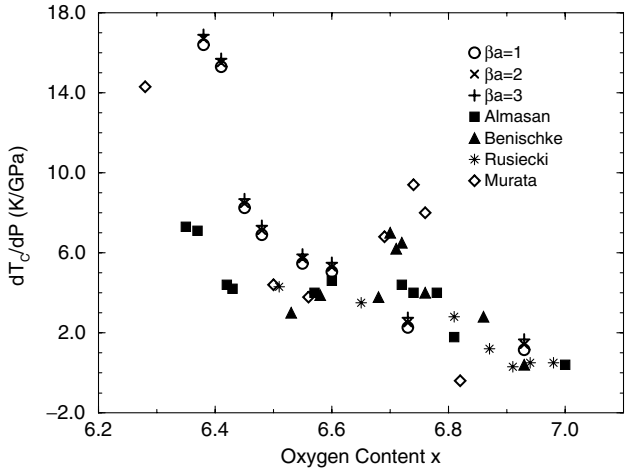

FIG. 2. Predicted variation of dT_c/dP with the oxygen stoichiometry x in $YBa_2Cu_3O_x$ for $\beta a = 1$, 2, and 3.

and it does not display a peak near $x \approx 6.7$ as observed by Murata *et al.* [26] and Benischke *et al.* [27]. However, a decreasing dT_c/dP with increasing T_c in $YBa_2Cu_3O_{7-\delta}$, one feature of our theoretical calculations, was observed experimentally by another group [29]. These discrepancies seem to be substantial for underdoped samples and it is therefore necessary to make more efforts from both experimental and theoretical sides to draw quantitative comparisons. Recently, it became apparent that the physics of underdoped cuprate superconductors is governed by another energy scale, the pseudogap [30]. Since the presence of the pseudogap above T_c, one expects that the pressure dependence of the pseudogap could play an important role in the pressure effect of T_c. Thus, the BCS-like equation for T_c may be inadequate for underdoped cuprates. In the present approach, it can be seen from Fig. 2 that the values of βa have little influence on the initial pressure derivative of T_c. Therefore it suggests that the behavior of dT_c/dP is dominated by the pressure-induced change of hole concentration in $YBa_2Cu_3O_{7-\delta}$ cuprates.

The double Cu-O chain compound $YBa_2Cu_4O_8$ has attracted a great deal of attention due to its excellent thermal stability, especially the large increase of T_c under hydrostatic pressure [31,32], in contrast to $YBa_2Cu_3O_7$. The higher pressure derivative of T_c found in this compound has been believed to originate from a much larger transfer of holes from the double chains to the CuO_2 planes, which has been confirmed by the study of chemical pressure via Ca substitution of the Y site in the parent compound [33], measurement of Hall effect under pressure [5], and calculation of Madelung energies [34]. Scholtz *et al.* [32] have determined that $d\ln n_H/dP = (9.8 \sim 18)\kappa_v$ by measuring both the T_c and the upper critical field H_{c2} from resistivity. The volume compressibility κ_v is taken to be 8.5×10^{-3} GPa^{-1} in $YBa_2Cu_4O_8$ from the structural changes under high pressure [34]. From Eqs. (1)–(3), one obtained the resulting value of hole concentration $n_H = 0.114$ holes corresponding to $T_c = 80$ K for the $YBa_2Cu_4O_8$ compound. The hole concentration n_H increases with pressure at a rate of $(9.5 \sim 17.4) \times 10^{-3}$ holes/GPa. It is reasonable to take $dn_H/dP = 1.4 \times 10^{-2}$ holes/GPa for the $YBa_2Cu_4O_8$ compound.

Choosing the lattice compressibility $\kappa_a = 3.0 \times 10^{-3}$ GPa^{-1} [34], one then evaluated the change of T_c with increasing pressure from 0 to 20 GPa in $YBa_2Cu_4O_8$ for coefficients $\beta a = 1$, 2, and 3. Results are presented in Fig. 3 and we see that the calculated $T_c(P)$ values agree with experiments [2,29,31,32,35] quantitatively. It should be noted that the agreement is achieved without introducing additional parameters. Thus, the theoretical approach introduced in this work offers a reasonable interpretation for the pressure dependence of T_c in $YBa_2Cu_3O_{7-\delta}$ and $YBa_2Cu_4O_8$. Good agreement with experiments indicates that the in-plane lattice parameter dependence of V_{eff} obeys $d\ln V_{\text{eff}}/d\ln a = -4 \sim -2$ for the Y-Ba-Cu-O

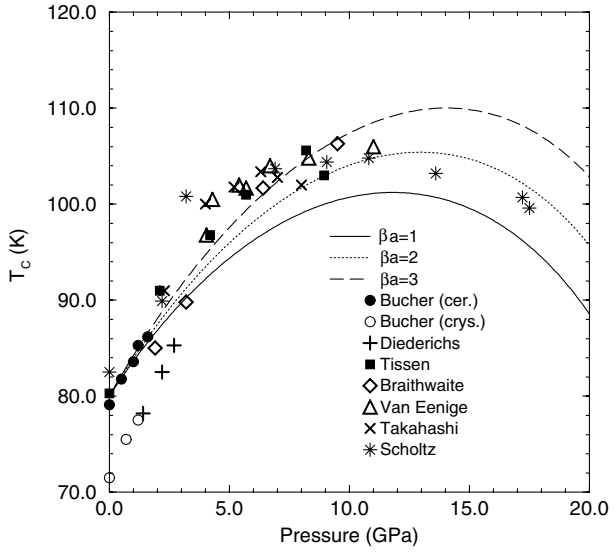

FIG. 3. Calculated values of T_c with pressure P in the $YBa_2Cu_4O_8$ compound with $T_c = 80$ K up to 20 GPa for $\beta a = 1$, 2, and 3.

system. Comparing to $d\ln K/d\ln a = +7.5$ for the transition metals in the conventional superconductors [20], our results indicate that the pairing mechanism of high-T_c superconductors seems to be different from that of the conventional superconductors. As shown by our results, the present approach is not sensitive to the specific form of V_{eff}. In fact, if one writes $T_c \approx M^{-\alpha}$ (α is the oxygen isotope exponent) and adopts the relation [20] that $d\ln K/d\ln v = 10(\alpha - 0.25)$, then from our results of $1 < \beta a < 3$ we would have $0.117 < \alpha < 0.183$, consistent with experimental data for optimally doped high-T_c superconductors [36]. Thus our approach is a simple but powerful tool for studying the pressure dependence of T_c in hole-doped HTSCs.

In summary, we have investigated both the variation of dT_c/dP with oxygen content in $YBa_2Cu_3O_{7-\delta}$ and changes of T_c with pressure in the $YBa_2Cu_3O_7$ and $YBa_2Cu_4O_8$ compounds by introducing two intrinsic variables, $n_H(P)$ and $V_{\text{eff}}(P)$, and solve BCS equations (1)–(3) with $d_{x^2-y^2}$ symmetry of order parameter. Our calculated results are in good agreement with experiments.

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