

Relationship between pressure-induced charge transfer and the superconducting transition temperature in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ superconductors

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A model is proposed for the pressure dependence of T_c based on the inverted parabolic relationship between T_c and the hole carrier density n that takes into account the fact that T_c drops to zero for a minimum value n^{\min} or a maximum value n^{\max} of n . The models proposed previously by Almasan *et al.* and Neumeier and Zimmermann are recovered, and are shown to be quite similar. Detailed calculations for $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ superconductors show that one can obtain large enhancements in T_c under pressure in materials that are highly underdoped, or have relatively modest rates of pressure-induced charge transfers. On the other hand, T_c enhancements in compounds which are near optimum doping or which have large rates of pressure-induced charge transfers are found to be quite modest.

I. INTRODUCTION

Considerable effort has been devoted in recent years to understanding the pressure dependence of the superconducting transition temperature T_c in the high-temperature cuprate superconductors,¹⁻⁷ with essentially two motivations; (1) to elucidate the mechanisms responsible for the high-temperature superconductivity, and (2) to find new materials with higher critical temperatures by using chemical pressure by means of chemical substitutions which mimic the effect of a true pressure. In the $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ family of superconductors, T_c varies strongly⁸ with the oxygen content δ and the highest values of T_c are obtained only for the nearly stoichiometric samples ($\delta \sim 0$). For oxygen-deficient samples ($\delta > 0.2$), T_c degrades rapidly until the material becomes an antiferromagnetic insulator for $\delta > 0.65$. It is noteworthy, however, that for oxygen-deficient samples with low- T_c values, one can obtain transition temperatures under pressure that exceed substantially those obtained on fully oxygenated samples.⁸⁻¹⁰

It is now well established that the holes created in the two-dimensional CuO_2 planes are responsible for superconductivity in the cuprate superconductors.¹¹ In the $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ family of superconductors the holes are created through the electron transfer from the CuO_2 planes to the CuO chains that act as electron reservoirs. Due to the structural changes under pressure there are subtle modifications in the electronic structure¹² that in turn change the charge-transfer interplay between the CuO_2 planes and the electron reservoirs CuO chains in the $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ family of superconductors. This clearly also results in a modification in the hole density in the CuO_2 planes. Several models^{1-4,6,7} have been proposed recently to account for the pressure dependence of T_c in terms of this pressure-induced charge transfer (PICT). In an interesting paper Almasan *et al.*⁶ presented recently a

pressure-induced charge-transfer model (PICTM) for the pressure dependence of T_c in the $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ family of superconductors which allowed them to obtain the magnitude of PICT as a function of δ . They found that the value of PICT is not constant but varies with δ . Interestingly, they also found that PICT displays a pronounced peak in the region of $\delta \sim 0.2$. The pressure-induced charge transfer clearly depends upon the underlying crystal structure and although large values of charge transfers *a priori* cannot be excluded, yet a very dramatic increase in charge transfer in a narrow domain of δ remains puzzling. In this paper we show that the magnitude of this peak is sharply reduced by a slight modification of their model in a way so that the variation of T_c with the hole concentration is better represented. However, the pronounced nature of PICT remains intact. The plan of this paper is as follows. In Sec. II the model for the dependence of T_c on the hole concentration is presented, and compared with the one given by Almasan *et al.*⁶ and by Neumeier and Zimmerman.⁷ The results for PICT are presented in Sec. III for $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ superconductors as a function of δ . Section IV is devoted to a calculation of T_c and dT_c/dP as a function of pressure P for several values of δ , and it is shown that strong T_c enhancement under pressure essentially occurs for underdoped compounds. The compounds that are near the optimum doping level are much less affected by pressure. It is also shown that, within this model, dT_c/dP is not constant but declines with pressure P , assuming a linear relationship between PICT and P , and this leads to the saturation and then a decline in the value of T_c under pressure. Concluding remarks are given in Sec. V.

II. MODEL

It is now well known that the superconducting transition temperature T_c in the cuprate superconductors

varies approximately in an inverted parabolic manner¹¹ with the hole concentration n in the CuO_2 planes. The compounds are nonmetallic and nonsuperconducting until a certain minimum concentration n^{\min} of holes is obtained in the CuO_2 planes. The T_c then begins to rise with increasing n and reaches a maximum value T_c^{\max} when an optimum concentration of holes n^{opt} is attained. For still larger values of n , the T_c again begins to decline and drops to zero for $n = n^{\max}$ in which case the compound behaves as a normal metal. This behavior can be expressed by a simple equation

$$T_c = \alpha(n - n^{\min})(n^{\max} - n), \quad (1)$$

for $n^{\min} \leq n \leq n^{\max}$. Here α is a constant. The maximum value of T_c will be obtained for a value of n where $dT_c/dn = 0$. This allows us to obtain the optimum value n^{opt} for n and the value of T_c^{\max} . These are given by

$$n^{\text{opt}} = (n^{\min} + n^{\max})/2, \quad (2)$$

and

$$T_c^{\max} = \alpha[(n^{\max} - n^{\min})/2]^2. \quad (3)$$

Combining Eqs. (1)–(3), one can write

$$T_c = T_c^{\max}[1 - \beta(n^{\text{opt}} - n)^2], \quad (4)$$

where

$$\beta = 1/(n^{\text{opt}} - n^{\min})^2. \quad (5)$$

This expression for T_c has been given previously.^{4,13,14} However, its implications for describing the pressure dependence of T_c have not been discussed before.

Following the works of Griessen and Wijngaarden and collaborators³ and Almasan *et al.*,⁶ Eq. (4) can be generalized to include the effect of pressure P

$$T_c(P) = T_c^{\max}(P)\{1 - \beta[n^{\text{opt}} - n(P)]^2\}, \quad (6)$$

where

$$n(P) = n + \Delta n(P)$$

and

$$T_c^{\max}(P) = T_c^{\max} + \Delta T_c^{\max}(P). \quad (7)$$

Here $n(P)$ and $T_c^{\max}(P)$ are the values of n and T_c^{\max} at pressure P , and n and T_c^{\max} their values at $P = 0$. According to Eq. (6), the change in the value of T_c at a given pressure occurs from two sources; (1) the pressure-induced change in the hole concentration $\Delta n(P)$, and (2) the change ΔT_c^{\max} in the value of T_c^{\max} that occurs due to other reasons, such as electron-phonon interaction, the coupling between the CuO_2 planes, etc., that are directly related to the mechanism responsible for the superconductivity. Note from Eq. (6) that $\Delta n(P)$ does not affect the value of $T_c^{\max}(P)$. In the absence of any detailed information concerning the behaviors of $\Delta T_c^{\max}(P)$ and $\Delta n(P)$ as a function of pressure, one can assume^{6,7} that they vary linearly with P , and write

$$\Delta T_c^{\max} = \alpha_1 P, \quad (8)$$

and

$$\Delta n(P) = \alpha_2 P, \quad (9)$$

where

$$\alpha_1 = \frac{dT_c^{\max}(P)}{dP} \quad (10)$$

and

$$\alpha_2 = \frac{dn(P)}{dP}. \quad (11)$$

Here α_1 and α_2 are constants independent of P . This approximation is reasonable for low values of P , but is likely to breakdown for large P since one expects $n(P)$ and $T_c^{\max}(P)$ to saturate at large pressures.

We can rewrite Eq. (6) so that the contributions to $T_c(P)$ from $\Delta T_c^{\max}(P)$ and $\Delta n(P)$ are separated:

$$T_c(P) = T_c + \frac{T_c}{T_c^{\max}} \Delta T_c^{\max}(P) + T_c^{\max}(P)\beta[2(n^{\text{opt}} - n) - \Delta n(P)]\Delta n(P). \quad (12)$$

As stated before T_c , T_c^{\max} , and n are their respective values at $P = 0$. In Eq. (12) the second term gives the contribution purely from the change in T_c^{\max} . Despite the appearance of $T_c^{\max}(P)$ in the third term, this last term is directly related to $\Delta n(P)$ and thus reflects essentially the contribution from the PICT.

From Eq. (6) one can also calculate $dT_c(P)/dP$, and this is given by

$$\frac{dT_c(P)}{dP} = \frac{T_c(P)}{T_c^{\max}(P)} \frac{dT_c^{\max}(P)}{dP} + T_c^{\max}(P)2\beta[n^{\text{opt}} - n - \Delta n(P)] \frac{dn(P)}{dP}. \quad (13)$$

Alternatively using Eqs. (10) and (11),

$$\frac{dT_c(P)}{dP} = \alpha_1 \frac{T_c(P)}{T_c^{\max}(P)} + 2\alpha_2\beta T_c^{\max}(P)[n^{\text{opt}} - n - \alpha_2 P]. \quad (14)$$

Here the first term reflects essentially the contribution from ΔT_c^{\max} , while the second term arises from $\Delta n(P)$.

The expression for $T_c(P)$ used by Almasan *et al.*⁶ is quite similar to our Eq. (6), and has the following form in our notation:

$$T_c(P) = T_c^{\max}(P) - \alpha[n^{\text{opt}} - n(P)]^2, \quad (15)$$

where α is a constant independent of P . However, α is determined from the fact that at $P = 0$, $T_c = 0$ for $n = n^{\min}$ ($n^{\min} = 0$ in the model of Almasan *et al.*), and thus

$$\alpha = T_c^{\max}/(n^{\text{opt}} - n^{\min})^2. \quad (16)$$

With this value one recovers our Eq. (4) for T_c at $P = 0$. Since α is directly related to T_c^{\max} , it seems natural that it obeys the same pressure dependence as T_c^{\max} , which leads to our Eq. (6) for $T_c(P)$. This leads to two minor

differences in the expressions (12) and (13) for $T_c(P)$ and $dT_c(P)/dP$. The corresponding expressions with α independent of pressure are the following:

$$T_c(P) = T_c + \Delta T_c^{\max}(P) + T_c^{\max}\beta[2(n^{\text{opt}} - n) - \Delta n(P)]\Delta n(P), \quad (17)$$

and

$$\frac{dT_c(P)}{dP} = \frac{dT_c^{\max}(P)}{dP} + T_c^{\max}2\beta[n^{\text{opt}} - n - \Delta n(P)]\frac{dn(P)}{dP}. \quad (18)$$

Thus the pressure dependence of α leads to a scaling of the contribution from the pressure dependence of T_c^{\max} . Further, the contribution from the PICT term also includes a slight effect from the variation of $T_c^{\max}(P)$ with P . However, these differences are clearly very minor when the T_c is near its optimum value. On the other hand, the contribution from the first term in Eq. (14) in the underdoped samples in the $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ superconductors is much smaller than the one from the second. Thus, one expects nearly the same results from Eq. (14) as obtained by Almasan *et al.* from Eq. (18) for the same set of parameters.

It should be noted that Eq. (17) for $T_c(P)$ and Eq. (18) for $dT_c(P)/dP$ are identical to the ones given by Neumeier and Zimmermann,⁷ which shows the unifying feature of our approach. However, there is one major difference in their interpretation. The first term in Eq. (17) corresponds to the true value of T_c at $P=0$ for the compound with n holes, and *not* the value of T_c for $\text{YBa}_2\text{Cu}_3\text{O}_7$. Neumeier and Zimmermann, in contrast, identify this term with the value of T_c for $\text{YBa}_2\text{Cu}_3\text{O}_7$ at $P=0$ for all compounds independent of their level of doping. This means that at $P=0$ one does not recover the true value of T_c for an overdoped or an underdoped compound in their model, which is clearly incorrect.

III. PRESSURE-INDUCED CHARGE TRANSFER

Due to the presence of $\Delta n(P)$ in the second term in Eq. (13), $dT_c(P)/dP$ clearly depends upon P . However, in the limit $P \rightarrow 0$ this term can be neglected so that

$$\frac{dT_c(P)}{dP} = \frac{T_c(P)}{T_c^{\max}(P)} \frac{dT_c^{\max}(P)}{dP} + T_c^{\max}(P)2\beta[n^{\text{opt}} - n] \frac{dn}{dP}, \quad (19)$$

which is similar to the expression used by Almasan *et al.* for the calculation of dn/dP .

In the $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ family of superconductors, an abrupt onset of superconductivity occurs⁶ for a hole density $n \sim 0.06$ hole/ CuO_2 and the maximum T_c is attained at a value of $n^{\text{opt}} \sim 0.25$ hole/ CuO_2 , so that $n^{\text{min}} = 0.06$ and $n^{\text{opt}} = 0.25$. From Eq. (5) we therefore obtain $\beta = 27.7/\text{hole}^2$.

Following Almasan *et al.* we assume $T_c^{\max} = 94$ K and $n = 0.257$ hole/ CuO_2 for fully oxygenated $\text{YBa}_2\text{Cu}_3\text{O}_7$.

This yields a $T_c = 93.873$ K for $\text{YBa}_2\text{Cu}_3\text{O}_7$ from Eq. (4), in agreement with the value of Almasan *et al.*

In a previous calculation¹⁵ an increase in the hole density of 0.0020 hole/ CuO_2 was obtained for $\text{YBa}_2\text{Cu}_3\text{O}_7$ at a pressure of $P = 0.578$ GPa. This gives $dn/dP = 3.46 \times 10^{-3}$ hole/GPa for $\text{YBa}_2\text{Cu}_3\text{O}_7$, in excellent agreement with the value given by Almasan *et al.*

From the work of Almasan *et al.*, we assume $dT_c/dP = 0.40$ K/GPa for $\text{YBa}_2\text{Cu}_3\text{O}_7$. From Eq. (19) we therefore obtain $\alpha_1 = dT_c^{\max}/dP = 0.527$ K/GPa. Almasan *et al.* obtained a value of $\alpha_1 = 0.48$ K/GPa. Thus our value is slightly higher. This difference arises from the fact that Almasan *et al.* have chosen $n^{\text{min}} = 0$ rather than the true value $n^{\text{min}} = 0.06$ hole/ CuO_2 .

With these parameters we can calculate from Eq. (19) the value of $\alpha_2 = dn/dP$ as a function of δ for $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ ($x = 7 - \delta$) superconductors using the T_c and dT_c/dP values given by Almasan *et al.* In Figs. 1 and 2 we have presented the values of T_c and dT_c/dP from Almasan *et al.* and the calculated values of n and dn/dP as a function of the stoichiometry δ in oxygen. We see from Fig. 2 that our calculated values of dn/dP are in fairly good agreement with those of Almasan *et al.* in two regions: (1) near the optimum doping, and (2)

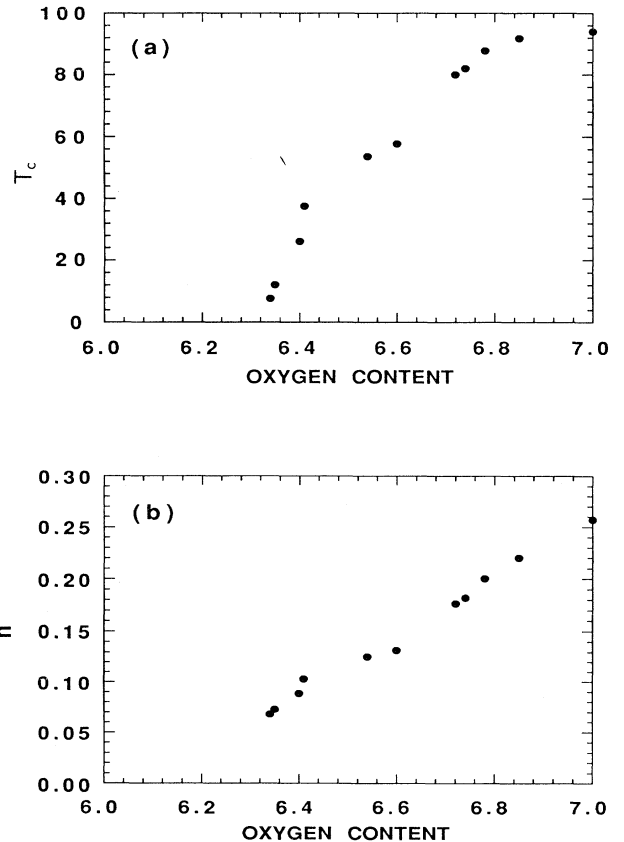


FIG. 1. Variation of (a) the superconducting transition temperature T_c (in K) from Almasan *et al.*, and (b) the hole density n per CuO_2 calculated from Eq. (4) as a function of the oxygen stoichiometry x in $\text{YBa}_2\text{Cu}_3\text{O}_x$.

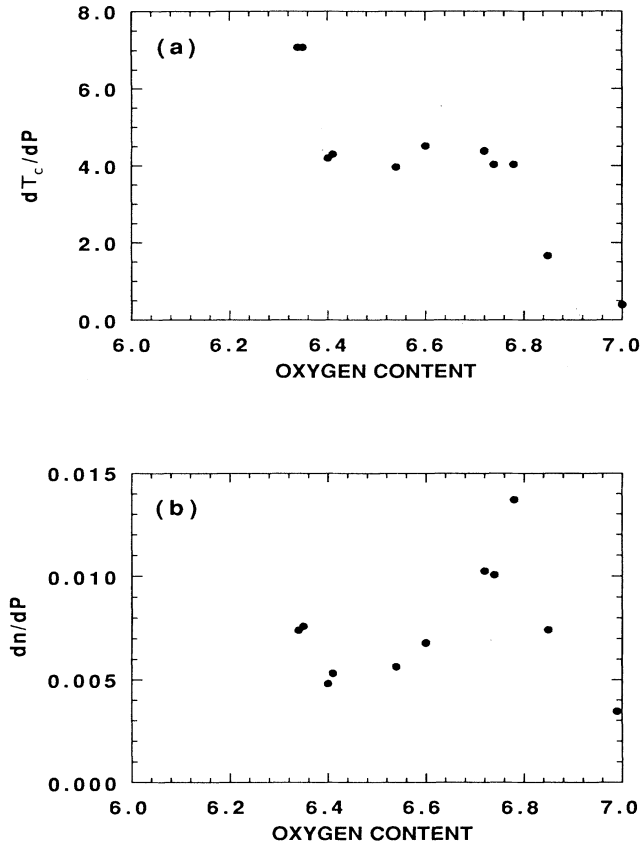


FIG. 2. Variation of (a) dT_c/dP (in K/GPa) from Almasan *et al.*, and (b) dn/dP (per CuO₂/GPa) calculated from Eq. (19) as a function of the oxygen stoichiometry x in YBa₂Cu₃O _{x} .

when the compound is highly underdoped with the oxygen content below 6.6. In the intermediate region, our values are substantially lower (by a factor varying between 1.3 and 1.6) than those obtained by Almasan *et al.*⁶ In particular, we obtain a maximum value of $dn/dP = 13.7 \times 10^{-3}$ hole/GPa for an oxygen content $x = 6.78$ with a T_c value of 87.6 K. This is smaller by a factor of ~ 1.6 from the value of $dn/dP \sim 22 \times 10^{-3}$ hole/GPa given by Almasan *et al.* For $x \sim 6.5$ we obtain a value of $dn/dP \sim 6 \times 10^{-3}$ hole/GPa, which is in good agreement with the value of $dn/dP \sim 6.9 \times 10^{-3}$ hole/GPa obtained from the electronic-structure calculations.¹⁶ The discrepancy between our results and those of Almasan *et al.* can be traced to their use of the value of n^{\min} . In their work they chose $n^{\min} = 0$, which from Eq. (5) yields a value of $\beta = 16.0/\text{hole}^2$. This has to be compared to our value of $\beta = 27.7/\text{hole}^2$ obtained with $n^{\min} = 0.06$ hole/CuO₂. Thus our value of β is a factor of 1.73 larger than the one obtained in the model of Almasan *et al.* This larger value of β has two effects: (1) one obtains from Eq. (4) a larger value of n , and hence a smaller value of $(n^{\text{opt}} - n)$, for the same value of T_c for underdoped samples, and (2) it tends to depress the value of dn/dP in Eq. (19) for the same value of dT_c/dP . In the highly underdoped region with $x < 6.6$, the two

effects in Eq. (19) nearly compensate. In the optimal doping region also, the value of dn/dP is not much affected since a larger value of β is compensated by a larger value of dT_c^{max}/dP , obtained for the same reasons. The largest change occurs in the intermediate region since the decrease in the value of $(n^{\text{opt}} - n)$ is relatively small ($\sim 10\%$) and cannot compensate for the very large increase in the value of β . This leads to a dramatic decrease in the value of dn/dP .

IV. VARIATION OF T_c AND dT_c/dP WITH P

Before presenting the results of detailed calculations for $T_c(P)$ and $dT_c(P)/dP$ for a few representative stoichiometries in oxygen (that define the starting hole concentrations) in YBa₂Cu₃O _{$7-\delta$} superconductors, a few general remarks are in order. We first notice from Eq. (6) that $T_c(P)$ cannot exceed $T_c^{\text{max}}(P)$, and this value is obtained when an optimum hole density under pressure, $n(P) = n^{\text{opt}}$, has been attained in the CuO₂ planes. Clearly, if $T_c^{\text{max}}(P)$ saturates and reaches a plateau when $n(P) = n^{\text{opt}}$, the maximum value of $T_c(P) = T_c^{\text{max}}(P)$ will be attained at this pressure P . A further increase in pressure will result in a decline in the value of $T_c(P)$ due to overdoping. On the other hand, if $T_c^{\text{max}}(P)$ has not reached a plateau and is still increasing with P in this range of pressure, the maximum value of $T_c(P)$ will be obtained *not* for $n(P) = n^{\text{opt}}$ but in a slightly overdoped region at a higher pressure at which the increase in $T_c(P)$ due to $T_c^{\text{max}}(P)$ [see Eq. (12)] is compensated by a decrease due to overdoping. Assuming $T_c^{\text{max}}(P)$ increases linearly with P , it is clear that the maximum T_c will be obtained for a compound in which the optimum hole density is achieved at very high pressures. This indicates that highly underdoped compounds are promising candidates for achieving large T_c enhancements under pressure, and the $T_c(P)$ values for these materials will significantly exceed the T_c values of the optimally doped compounds at normal pressures.

From Eq. (14) one sees that $dT_c(P)/dP$ is not constant but varies significantly with pressure. This fact has not been widely appreciated in the literature. Indeed, the variation of $dT_c(P)/dP$ with P can yield some information concerning the nature and the magnitude of the pressure-induced charge transfer $\Delta n(P)$. One also notices from Eq. (14) that the contribution of $\Delta n(P)$ to $dT_c(P)/dP$ is such that $dT_c(P)/dP$ has the maximum value at $P \rightarrow 0$ and declines with increasing P . For underdoped samples, the contribution from the $\Delta n(P)$ term remains positive until an optimum value of the total hole density under pressure has been obtained, i.e., $n(P) = n^{\text{opt}}$. A further increase in $n(P)$ makes its contribution negative. However, due to the contribution from the first term in Eq. (14) arising from the pressure dependence of T_c^{max} , $dT_c(P)/dP$ becomes negative only at higher pressures.

This behavior is reflected in the variation of $T_c(P)$ with P . From Eq. (12) one sees that the contribution to $T_c(P)$ from the $\Delta n(P)$ term in the underdoped compounds follows an inverted parabolic behavior. As $\Delta n(P)$ increases

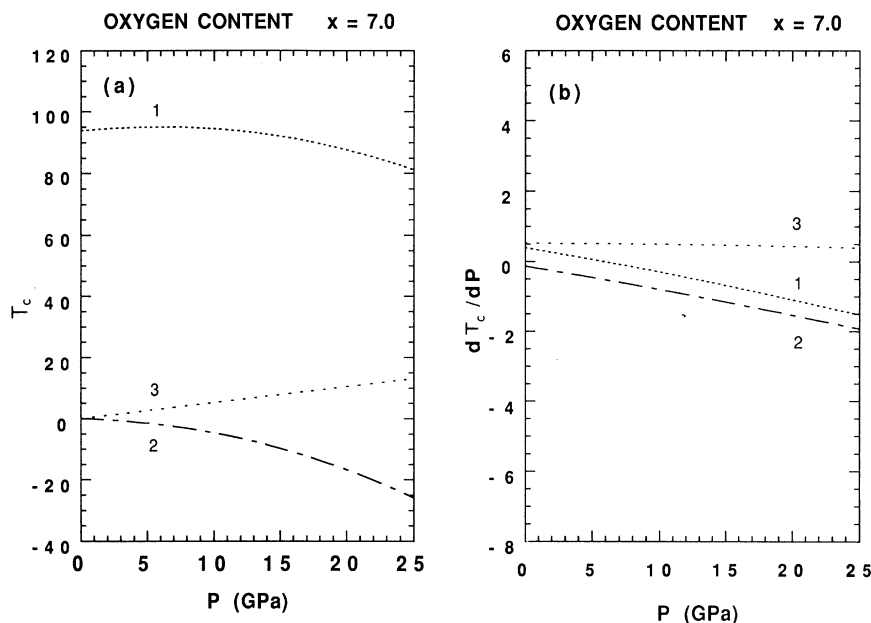


FIG. 3. Variation of T_c (in K) [(a), curve 1], and dT_c/dP (in K/GPa) [(b), curve 1] as a function of pressure P in YBa₂Cu₃O₇. Curves 2 and 3 represent the contribution from the pressure-induced charge-transfer PICT term and the variation of $T_c^{\max}(P)$ term with pressure, respectively, in Eqs. (12) and (14).

with P , the contribution from the PICT term increases and reaches a maximum when $n(P) = n^{\text{opt}}$, after which it begins to decline and becomes negative for values of $\Delta n(P) > 2(n^{\text{opt}} - n)$. The value of $T_c(P)$ reaches its maximum when $n(P) \sim n^{\text{opt}}$, and for higher pressures it begins to decline. It should also be noted from Eq. (12) that a large value of dn/dP is not very helpful in achieving larger values of $T_c(P)$, especially in superconductors which are near the optimum doping, since optimum hole densities are obtained at low pressures for which $T_c^{\max}(P)$ is not significantly different from its normal pressure value of T_c^{\max} . At higher pressures, the $T_c(P)$ in these compounds begins to drop quickly.

In Figs. 3–5 we have shown the variations of $T_c(P)$ and $dT_c(P)/dP$ with P for three different stoichiometries in oxygen using the parameters obtained above. Contributions from the $\Delta T_c^{\max}(P)$ and $\Delta n(P)$ terms are also shown in order to indicate their relative importance. Figure 3 shows the results for YBa₂Cu₃O₇ with $T_c = 93.873$ K and $n = 0.257$ hole/CuO₂, which has nearly the optimum hole density but slightly overdoped. The rate of the pressure-induced charge transfer in this compound is rather low, $dn/dP = 3.46 \times 10^{-3}$ hole/GPa. Due to the overdoped nature of this compound, the contributions from the $\Delta n(P)$ term to both $T_c(P)$ and $dT_c(P)/dP$ are negative. The increase in the value of $T_c(P)$ arises only

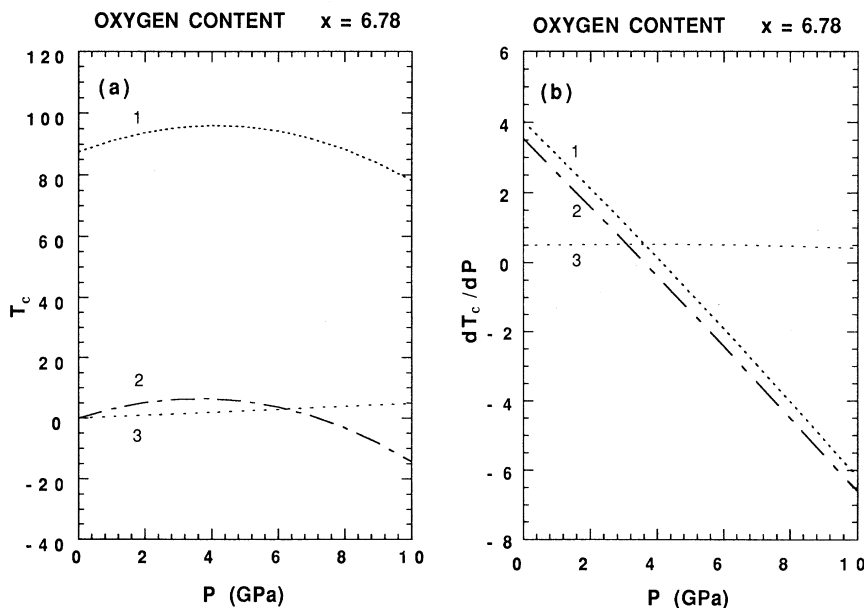


FIG. 4. Same as Fig. 3 for YBa₂Cu₃O_{6.78}.

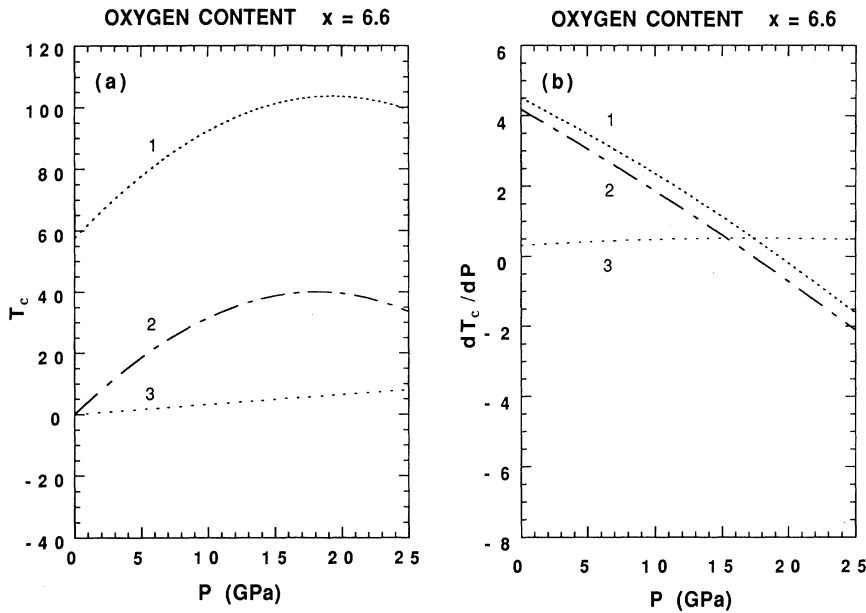


FIG. 5. Same as Fig. 3 for $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$.

due to an increase in the value of $T_c^{\text{max}}(P)$ which is rapidly compensated by a decrease due to $\Delta n(P)$, and only a very modest increase to $T_c(P)=95.09$ K is attained at 6 GPa. At higher pressures $T_c(P)$ begins to decline and reaches a value of 81.2 K at 25 GPa. With a larger value of dn/dP , even lower values of $T_c(P)$ and $dT_c(P)/dP$ would have been obtained at the same pressures. Due to the low value of dn/dP , the variation in $dT_c(P)/dP$ with P is rather small, especially at low pressures.

In Fig. 4 are presented the results for $\text{YBa}_2\text{Cu}_3\text{O}_{6.78}$ which has a T_c value of 87.6 K and a hole density $n=0.200$ hole/ CuO_2 . This compound is marginally underdoped but has a large value of PICT with $dn/dP=13.7 \times 10^{-3}$ hole/GPa. Due to this large charge transfer, $dT_c(P)/dP$ declines rapidly with P , and $T_c(P)$ attains its maximum value of 96.03 K at 4 GPa. At only 10 GPa the value of $T_c(P)$ has declined to 78.2 K, and $dT_c(P)/dP$ is highly negative with a value of -6.2 K/GPa. This indicates that with large values of dn/dP it is difficult to obtain large enhancements of T_c under pressure.

The results for $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$ are presented in Fig. 5. This compound has a $T_c=57.6$ K and is highly underdoped and has a hole density of $n=0.132$ hole/ CuO_2 . The value of PICT is intermediate between the first two cases with $dn/dP=6.80 \times 10^{-3}$ hole/GPa. Due to its highly underdoped nature and a modest value of dn/dP , the variation of $dT_c(P)/dP$ with P is much smaller, and $T_c(P)$ increases in a regular manner with P . It already attains 94 K, the maximum value for an optimally doped $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ compound ($\delta \sim 0.07$) at normal pressure, at $P \sim 10.5$ GPa and this is not its maximum. At higher pressures it considerably exceeds this value and the maximum is achieved for $P \sim 19$ GPa with $T_c(P) \sim 103.6$ K. This represents an increase of 80% over its value at normal pressure in this compound, and an increase of 10% of the value of the optimally doped $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ at nor-

mal pressure. It should also be noted that the maximum $T_c(P)$ in this compound far exceeds the maximum values of $T_c(P)$ obtained for the nearly optimally doped $\text{YBa}_2\text{Cu}_3\text{O}_7$ and the marginally underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{6.78}$ compounds.

V. CONCLUSION

We have derived in this paper an expression for T_c in terms of the hole carrier density n in the CuO_2 planes that has the form of an inverted parabola and correctly takes into account the fact that T_c attains its maximum value for an optimum number n^{opt} of holes in the CuO_2 planes and drops to zero when the hole density is below a critical threshold n^{min} or exceeds a maximum value n^{max} . This model presents a unifying feature in that the models presented earlier by Almasan *et al.*⁶ and Neumeier and Zimmermann⁷ are recovered, and are found to be essentially the same. We have also shown that the value of n^{min} can considerably affect the calculation of the rate of the pressure-induced charge transfer dn/dP from the measured values of dT_c/dP . With $n^{\text{min}}=0$ Almasan *et al.* obtained a large value of $dn/dP \sim 22.0 \times 10^{-3}$ hole/GPa for $\text{YBa}_2\text{Cu}_3\text{O}_{6.78}$. However, in the $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ family of superconductors, the threshold for superconductivity is observed at $n^{\text{min}} \sim 0.06$ hole/ CuO_2 . With this a considerably reduced value of $dn/dP=13.7 \times 10^{-3}$ hole/GPa is obtained for $\text{YBa}_2\text{Cu}_3\text{O}_{6.78}$.

We have also shown that, contrary to what one normally expects, $dT_c(P)/dP$ is not constant, even at low pressures. It is maximum for $P \rightarrow 0$ and declines with increasing P . The rate of this decline is intimately related to both the value of dn/dP and the value of n . The value of $dT_c(P)/dP$ decreases rapidly for large values of dn/dP . Detailed calculations show that large enhance-

ments in the value of T_c under pressure can be obtained for materials which are highly underdoped, and not for compounds which have nearly optimum or marginally optimum hole densities at normal pressures. The value of $T_c(P)$ in the highly underdoped materials and with reasonably modest values of dn/dP can far exceed the value of T_c at optimum doping at normal pressure.

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