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STUDY ON THE DEPENDENCE OF THE CRITICAL TEMPERATURE T_c ON PRESSURE IN $YBa_2Cu_3O_{6+x}$

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Abstract

In the present study experimental data available in the literature have been employed to investigate behavior of the critical temperature T_c as a function of the pressure P, in the $YBa_2Cu_3O_{6+x}$ high temperature superconductor (HTSC). We estimated the maximal critical temperature $T_{c,max}(P)$ which can be achieved in this material under pressure applied at temperatures low enough to prevent oxygen reordering. We found that it approximately equals to 114K corresponding to $x \approx 0.77$.

Introduction

Many studies conducted in the past years on the pressure effect in HTSC materials revealed the complex nature of the pressure dependence of T_c in these materials, since T_c depends on many different parameters such as hole carrier density, interplanar and intra planar spacing, relaxation parameters etc. [1,2]. It is usually assumed that two different terms contribute to the pressure coefficient (dT_c/dp), one, which results from the pressure induced charge transfer and the other, intrinsic one, which is not result of the charge transfer [3].

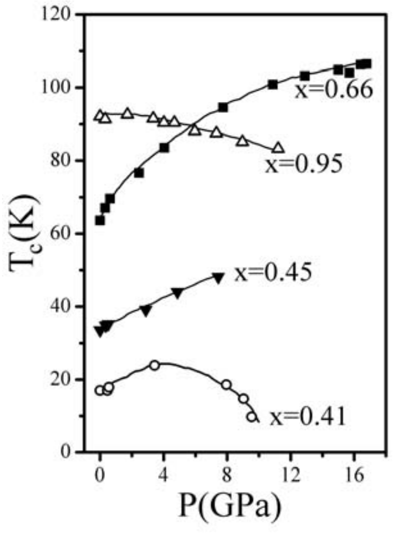

Fig.1. T_c as a function of pressure P for different oxygen concentrations x. The results are reproduced from the Ref. [4].

For the HTSC compounds with initially positive pressure coefficient, it is characteristic that the pressure increase leads to the enhancement of the T_c until, for some pressure P_{max}, the maximum T_c is reached, and at yet higher pressures T_c decreases again [4]. In $YBa_2Cu_3O_{6+x}$ material pressure coefficient considerably depends on the oxygen concentration x. For $x \approx 0.97$ the material is optimally doped and the pressure effect is almost negligible. For very under doped samples a giant pressure coefficients up to 30K/GPa was reported when the pressure was applied at room temperatures, while at 100K only moderate T_c increase was achieved (2-4K/GPa) [5]. The T_c enhancement at room temperature was attributed to the increased doping of CuO_2 planes achieved by the pressure induced oxygen reordering which is suppressed at low temperatures [5].

Results and discussion

Since the pressure application increases number of holes in the CuO_2 planes, there is a certain similarity between doping and pressure experiments. Therefore, the following relation is able to describe the T_c vs P behavior observed in many high-T_c cuprates [6]:

$$T_c(P) = T_{c,\max}\left[1 - A\left(P - P_{\max}\right)^2\right]. \quad (1)$$

In the present paper we have employed this relation to fit the experimental results of Sadewasser *et al* [4] who have measured the critical temperature T_c as a function of the hydrostatic pressure P, in $YBa_2Cu_3O_{6+x}$ over the wide range of oxygen concentrations x (figure 1) at temperatures which exclude the oxygen reordering. Then we presented the so obtained T_c values as a function of the concentration x at different P = *const* values, and fitted those $T_c(x)$ dependences to the parabolic curve as shown in the figure 2. Such an approximation was suggested by Stankowski *et al* [6] and it can be seen that the $T_c(x)$ values extracted from (1) for P = *const* are fitted by the parabolic approximation very well. However, we must note that it is not strictly valid in the whole range of oxygen concentrations since it does not includes 60K plateau displayed in the T_c vs. x characteristic at $P = 0$ for $0.5 < x < 0.63(3)$. From the fig. 2 (we showed the results only for two values of $P \neq 0$) it can be seen that with the pressure increase leads to the higher maximal T_c value and that it is achieved for samples with lower oxygen concentration x. This implies that at high pressures the optimal hole doping of CuO_2 planes is achieved for the samples with larger oxygen deficiency, such a behavior being the obvious consequence of the additional pressure induced charge transfer from CuO to the CuO_2 planes.

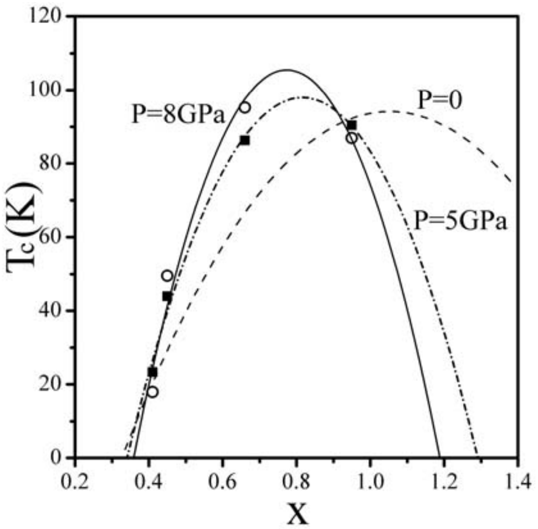

Fig. 2. T_c as a function of the oxygen content x at P=0 and under pressure for P=5GPa and P=8GPa. The lines are parabolic approximation to the experimental results taken from [3].

The parabolic approximation of the existing experimental results for $T_c(x)$ dependence at high constant pressures enabled determination of the $T_c(P)$ dependences for the samples in the wide range of oxygen concentrations where experimental results are available. For those samples, which do not reach their maximal T_c values for pressures that are too high, the equation (1) is used to determine their maximal T_c under pressure. We presented this way estimated maximal T_c values as well as those determined experimentally a function of the concentration x in the figure 3. We found that this dependence can be also, to a very good approximation fitted to the parabolic curve. This way the maximal T_c under pressure, can be determined for the whole range of concentrations x where the material behaves as a superconductor.

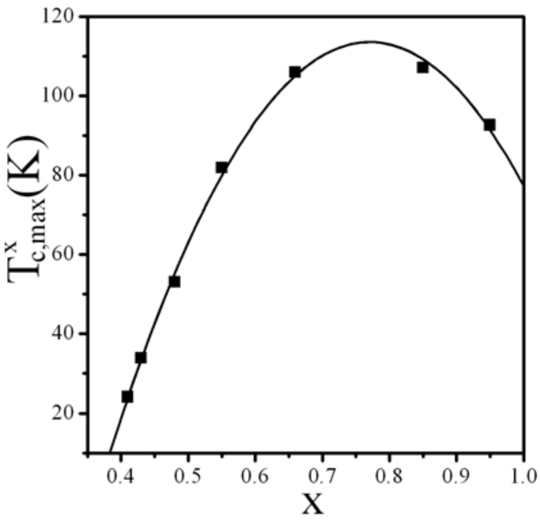

Fig. 3. Maximal T_c which can be achieved in the sample under pressure as a function of the concentration x.

Conclusion

We estimated the maximum T_c, that can be achieved under pressure at low temperatures in $YBa_2Cu_3O_{6+x}$ HTSC, to be approximately 114K, and it is reached for $x \approx 0.77$, which is the concentration close to the one at which the maximal pressure coefficient is measured [5]. However, it was not possible to determine the value of the pressure at which this maximum T_c is reached, though our analyses indicate that it is around 9GPa. For more precise estimation, high pressure experimental results for T_c obtained on the larger set of samples with different oxygen contents are needed.

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References

[1] J. S. Schilling, Treatise on High Temperature Superconductivity, ed. by J. R. Schrieffer, Springer, Verlag, 2006, 427-462.

[2] B. Lorenz, C. W. Chu, Frontiers in superconducting materials, Springer Berlin Heidelberg, 2005, 459-497.

[3] J. J. Neumeier, H. A. Zimmerman, Phys. Rev. B, 1993, **47**, 8385.

[4] S. Sadewasser, J. S. Schilling, A. P. Paulikas, B. W. Veal, Phys. Rev. B, 2000, **61**, 741-749.

[5] W. H. Fietz, R. Quenzel, H. A.Ludwig, K. Grube, S. I. Schlachter, F. W. Hornung, T. Wolf, A. Erb, M. Klaser, G. Muller-Vogt, Physica C, 1996, **270**, 258-266.

[6] J. Stankowski, M. Krupski, R. Micnas, Mater. Sci. Poland, 2004, **22**, 175-185.