Hydrostatic and Uniaxial Pressure Effect on T_c of $YBa_2Cu_3O_X$

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The variation of the transition temperature T_c of $YBa_2Cu_3O_x$ with hydrostatic He-gas pressure depends on the oxygen content x. The pressure effect dT_c/dp increases from small negative values at x=7 to dT_c/dp=7.4 K/GPa at x=6.7. For oxygen contents below x=6.7 dT_c/dp drops to 3 K/GPa and remains nearly constant[1]. The charge transfer model[2] cannot explain the drop at x=6.7.
Thermal expansion measurements on $YBa_2Cu_3O_x$ indicated that the uniaxial pressure effects along the three crystal axes are different[3,4]. To investigate the uniaxial pressure effects inductively an experimental setup was constructed. The T_c-change of several $YBa_2Cu_3O_x$ single crystals with different oxygen contents has been investigated under pressure along the c-axis. To avoid oxygen ordering processes the samples were held below 105 K during the measurements. The results of uniaxial pressure measurements in c-axis direction fit to former uniaxial pressure data[3,4,5] and are explained within the charge transfer model. Hydrostatic pressure data[12] of overdoped samples fit to the same curve. However, this is not the case for underdoped samples. From this we conclude that only a part of the hydrostatic pressure effect can be explained by charge transfer in the underdoped region. The remaining part can be ascribed to uniaxial pressure effects along the a- and b-axis.

1. INTRODUCTION

In many experiments $YBa_2Cu_3O_x$ serves as a model for high temperature superconductors. T_c of $YBa_2Cu_3O_x$ can be varied continuously from zero to 93 K by annealing in an appropriate atmosphere to adjust the oxygen content and change hereby the hole concentration n_h. By partly substituting Ca for Y, n_h can be increased further which reduces T_c in the overdoped region. It is generally accepted that $T_c(n_h)$ has a parabolic shape for most HT_cSC's[6], but the maximum T_c is limited to different $T_{c,max}$ for different materials. For a given structure T_c cannot only be changed by oxygen and Ca doping, but also by hydrostatic pressure which increases n_h, too. In contrast to chemical doping, pressure allows to vary T_c without changing the chemical composition. Therefore, pressure experiments are a good choice to investigate the variation of T_c with n_h. If the n_h-increase under pressure dn_h/dp is nearly independent of n_h, dT_c/dp gives a measure for the derivative of the $T_c(n_h)$ curve:

$$\frac{dT_c(n_h)}{dp} = \frac{dT_c}{dn_h} \cdot \frac{dn_h}{dp} = \frac{dT_c}{dn_h} \cdot const. \tag{1}$$

If $T_c(n_h)$ has a parabolic shape dT_c/dp is proportional to n_h and, therefore, a qualitative measure for the hole concentration[1,7]. Hydrostatic pressure experiments showed two problems with this explanation: First, dT_c/dp is not exactly zero for optimal doping, i.e., maximal T_c, and second, dT_c/dp drops at x=6.7 from 7.4 K/GPa to 3 K/GPa for decreasing oxygen content x.

The hydrostatic pressure effect can be obtained by the sum of the uniaxial pressure effects along the three crystal axes. Therefore, uniaxial pressure experiments allow a more detailed investigation of the changes under pressure, possibly a separation of charge transfer effects from other effects.

2. EXPERIMENTAL

Fig. 1 shows the setup to investigate ac-susceptibility under uniaxial pressure. A bellow, loaded with Helium gas, supplies the uniaxial force, allowing a smooth pressure application to the brittle samples and pressure changes at low temperatures. The latter is important to have the possibility to avoid pressure induced oxygen ordering leading to a drastically enhanced pressure effect for oxygen deficient samples[8]. The pistons are kept parallel by a parallelogram spring suspension avoiding abrupt movements due to friction of the piston during pressure application. The pistons are sapphire cylinders that give no background signal. We selected this hard material, because smooth pistons would be deformed during the experiment resulting in an uncontrolled support of the sample perpendicular to the pressure axis. In this case the sample would be exposed to a mixture of the uniaxial pressures along all three crystal axes. The ac-susceptibility is measured by a compensated pickup coil system.

The change of T_c under uniaxial pressure has been measured on four $YBa_2Cu_3O_x$ single crystals. All samples were prepared as described in [9] using ZrO_2 crucibles. Sample 1 and 2 had dimensions of 0.90*1.24*0.12 mm^3 and 1.09*1.63*0.12 mm^3 with T_c of 77.5 K and 87.8 K, respectively. Sample 2

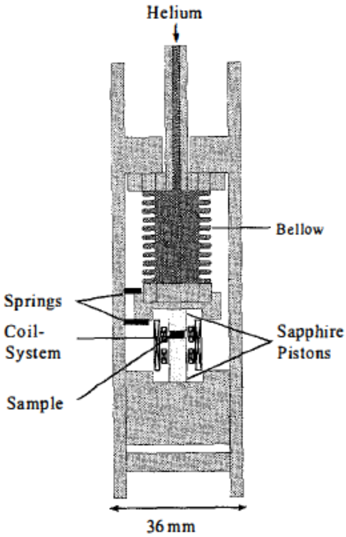

Fig. 1. The uniaxial pressure cell.

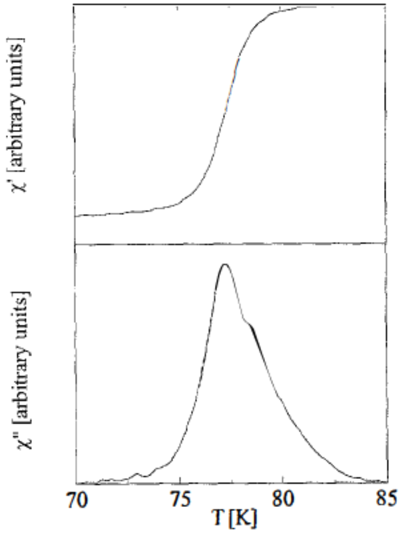

Fig. 2. χ' and χ'' of sample 1 measured at ambient pressure.

fractured at the highest pressure of 0.15 GPa. A part of this sample with the dimensions 0.80*1.63*0.12 mm^3 was tempered to get a T_c of 48.7 K and was labelled sample 3. Sample 4 was held 11 d at 380°C in flowing oxygen which results in an oxygen content of 6.99 according to Lindemer et al.[10]. The dimensions of this sample are 1.32*1.92*0.54 mm^3.

3. RESULTS

Fig. 2 shows the ac-susceptibility χ' and χ'' of sample 1 at ambient pressure. In fig. 3 χ' of sample 1 is shown measured at uniaxial pressures p_c of 0 GPa, 0.08 GPa and 0.15 GPa. The transition broadens slightly under pressure. By varying the parallelism of the ab-surfaces of a sample we found an increase of the broadening with increasing non-parallelism. Therefore, we attribute a broadening of the transition to an inhomogeneous pressure distribution due to not perfectly parallel ab-surfaces of the sample.

For a transition that broadens under uniaxial pressure in c-axis direction p_c, the resulting dT_c/dp_c value depends on the T_c criterion. Fig. 4 shows $T_{c,50\%}$ values of sample 1 increasing with pressure. Between 20% and 80% of the transition the broadening is weak and the dT_c/dp_c values for the different criteria give $dT_c/dp_c = 2.8$ K/GPa ± 0.5 K/GPa. Aside from this effect the accuracy of the dT_c/dp_c determination is limited by the uncertainty of the measurement of the sample dimensions which are needed to calculate the pressure applied to the

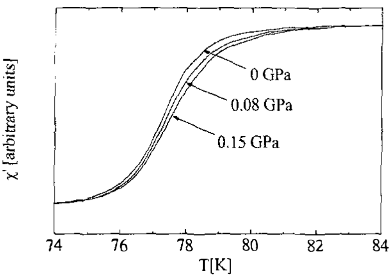

Fig. 3. ac-susceptibility of sample 1 measured at various uniaxial pressures p_c.

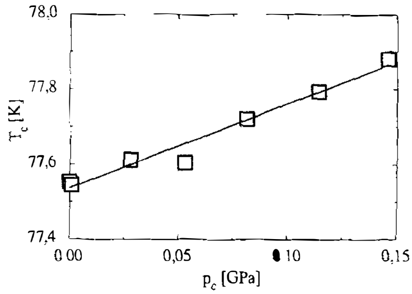

Fig. 4. $T_{c,50\%}$ of sample 1 versus uniaxial pressure p_c.

sample. This measurement can be done with an accuracy of about ± 5% depending on the sample geometry and the quality of the surfaces. The accuracies for determining χ', χ", T and p_{Helium} are better than ± 1%. For all investigated samples we estimate the error in dT_c/dp to be below ± 20% indicated by the error bars in fig. 5.

Fig. 5 shows dT_c/dp_c values in dependence on the initial $T_c(p=0)$ of the samples. The black solid squares show the results of our measurements. For comparison, values calculated from high-resolution thermal expansion measurements[3,4] and values from uniaxial pressure experiments[5] are shown. Fig. 5 also includes dT_c/dp values from hydrostatic pressure experiments[13,14] represented by the crosses. The dashed line is a guide for the eye for the hydrostatic data. The origin of the solid curve will be discussed later.

4. DISCUSSION

The charge transfer picture assumes that holes from the CuO-chains are transferred to the CuO_2-planes[2] under pressure. Usually, the position of the apical oxygen atom and the position of the Ba ion are thought to be responsible for the amount of transferred holes. Unfortunately, there are no experimental data available monitoring the atomic positions under uniaxial pressure. Therefore, an ionic model has been calculated to get a qualitative estimation of the change of the atomic positions under uniaxial pressure[11]. This model predicts a strong shift of the apical oxygen atom towards the CuO_2-planes and of the Ba ion towards the CuO-chains for pressure along the c-axis, resulting in a very effective charge transfer.

Assuming $T_c(n_h)$ being of parabolic shape and dn_h/dp_c being nearly constant for all oxygen contents we get for dT_c/dp_c

$$\frac{dT_c}{dp_c} = \sqrt{\frac{T_{c,\max} - T_c(p=0)}{\gamma}} + \alpha \frac{T_c(p=0)}{T_{c,\max}} . \tag{2}$$

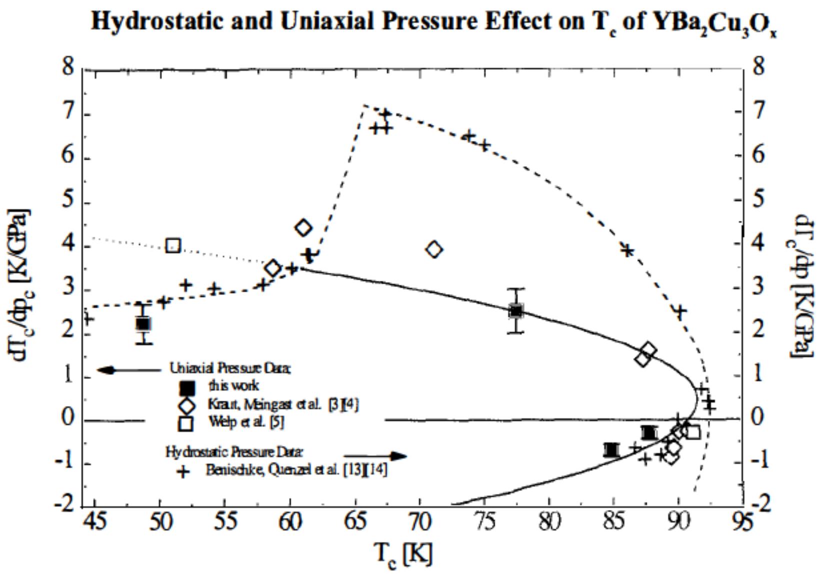

Fig. 5. Uniaxial (left axis) and hydrostatic pressure effects (right axis) in dependence on T_c at ambient pressure. The solid squares and the open symbols represent uniaxial pressure data. The solid curve is discussed in the text. The crosses give the values for the hydrostatic pressure effect[13,14] with the dashed line as a guide for the eye.

$T_{c,max}$ is the T_c for optimal oxygen doping and α, γ are constants. This is the same approach that was used to describe hydrostatic pressure experiments earlier[1]. The constants in (2) were adjusted to fit hydrostatic pressure experiments[12] on overdoped $(Y_{1-y}Ca_y)Ba_2Cu_3O_x$ single crystals and with these values equation (2) was used to calculate the solid curve in fig. 5. Surprisingly, the hydrostatic pressure data for underdoped samples do not fit to this curve[12] and follow the dashed line in fig. 5, but the data from c-axis pressure experiments fit the solid curve for over- and underdoped samples. Therefore, the T_c-change by hydrostatic pressure in the overdoped region can be explained by the effect of c-axis compression, only. As a consequence the difference of the solid and the dashed line in the underdoped region has to be attributed to uniaxial pressure effects in a- and b-axis direction. Especially, the sharp drop of the hydrostatic pressure effect has to be correlated to a change of the uniaxial pressure effects in a- and b-axis direction at x=6.7 which might be connected to the Ortho I / Ortho II transition. The uniaxial pressure effect in c-axis direction can be affected by this transition, too, which might explain the low dT_c/dp_c-value of sample 3 at 48.7 K. Therefore it is questionable if the solid parabola, which was calculated from the charge transfer model, can be extended below 60 K. Further investigations are necessary to decide whether a sharp change of dT_c/dp_c at x=6.7 is absent for the uniaxial pressure along the c-axis.

5. CONCLUSIONS

An experimental setup has been built to detect the T_c variation under uniaxial pressure by ac-susceptibility measurements. T_c of several $YBa_2Cu_3O_x$ single crystals with different oxygen contents has been investigated under uniaxial pressure along the c-axis. The effect of uniaxial pressure along the c-axis can be described within the charge transfer model which is consistent with hydrostatic pressure data[12] for overdoped samples. Hydrostatic pressure data[13,14] of underdoped samples do not fit to this model. From this we conclude that in the underdoped region only a part of the hydrostatic pressure effect, namely uniaxial pressure in c-axis direction, can be explained by charge transfer. The remaining part has to be ascribed to uniaxial pressure effects along the a- and b-axis with an increasing contribution to the hydrostatic pressure effect for decreasing oxygen content. Further investigations are necessary to find out, whether there is a change in the c-axis pressure effect at the Ortho I / Ortho II transition at x=6.7.

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