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VOLUME DEPENDENCE OF HIGH-T_c SUPERCONDUCTORS

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The pressure dependence of T_c is found to be large for the superconductors (La-Ba-Cu-O, La-Sr-Cu-O) with a relatively low T_c and small for Y-Ba-Cu-O. The implications of this trend for the theories of high-T_c superconductivity (especially those based on a Hubbard-like model) are discussed.

1. INTRODUCTION

Shortly after the publication of Bednorz and Müller (1) on superconductivity in La-Ba-Cu-O, Chu et al. (2) reported that the T_c of this compound could be increased from 32 K to 40 K by applying a hydrostatic pressure of 14 kbar. With dT_c/dp = 0.64 K/kbar La-Ba-Cu-O has one of the largest positive pressure dependence measured so far. On the other hand for Y-Ba-Cu-O Hor et al. (3) found a very weak pressure dependence of T_c up to 19 kbar. This behaviour was confirmed in our laboratory up to 170 kbar (4). For this investigation we used the same diamond-anvil-cell as Hemmes et al. (5) for the high pressure synthesis of superconducting stoichiometric PdH and PdD. The good agreement between the low-pressure and the high pressure data obtained by means of this diamond cell show that the low dT_c/dp is an intrinsic property of $Y_1Ba_2Cu_3O_7$.

2. TRANSITION

As shown in Fig. 1 both the low and high pressure data exhibit a small increase with pressure for the onset temperature T_{co} and a small decrease of T_{cf}, the temperature below which the sample is in the zero-resistivity state. The middle of the transition T_m is almost pressure independent while the transition width increases with 0.113 K/kbar. This large broadening cannot be explained in terms of pressure gradients present in the diamond anvil cell as $dT_m/dp \simeq 0$. It is more likely related to the presence of local uniaxial stresses due to the granular nature of the sintered samples used in this work. Using the simple model of Salomons et al. (6) we estimate that for a sample with a density of 80% of the single crystal density, at a pressure of 170 kbar, the c/a-ratio in the uniaxially stressed regions differ by 7.5% from that of the unstressed unit cell. As at 170 kbar the transition width is ~ 19 K we estimate that T_c increases (or decreases) by 1.3 K for a 1% change in c/a.

3. THEORETICAL MODELS

In Fig. 2 the relative volume dependence of T_c is shown as a function of T_c. There is a clear trend which cannot be understood within the classical BCS-theory. Bipolaronic superconductivity could in principle lead to large negative volume derivatives but would also predict large isotope effects in contradiction

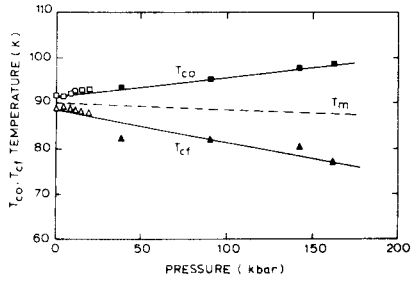

Fig. 1 Pressure dependence of T_c for $Y_1Ba_2Cu_3O_{\sim 7}$

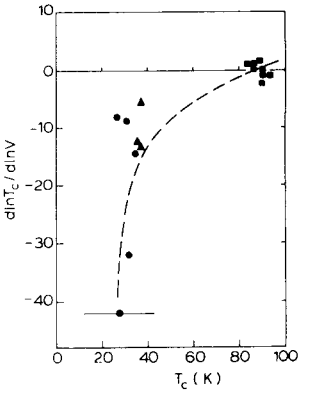

Fig. 2 Volume derivative of T_c as a function of T_c (for references see ref. 7)

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with available experimental data. The volume derivatives predicted by several theoretical models are discussed in ref. 7.

In the remaining part of this paper we present some implications of the data in Fig. 2 for theoretical models based on the Hubbard-Hamiltonian,

$$H = \sum_{i,j} t_{ij}\, c^{+}_{i\sigma}\, c_{j\sigma} + U \sum_{i} n_{i\uparrow}\, n_{i\downarrow} \qquad (1)$$

where U is the intra-atomic Coulomb integral and t_{ij} is the hopping integral between sites i and j. Depending on the approximations used and the additional terms considered by various authors in the hamiltonian indicated above, different expressions have been proposed so far for T_c. Some results are clearly incapable of giving large negative $d\ln T_c/d\ln V$. To illustrate this point we consider some specific types of expressions for T_c.

In general, T_c depends on t, U and the average number n of electrons (or holes) per site. From dimensional considerations one expects that,

$$T_c = (t^2/U) f(t/U, n) \qquad (2)$$

For La-Ba-Cu-O, La-Sr-Cu-O and Y-Ba-Cu-O band structure calculations lead to $t \cong 0.5$ eV and experiments on copperoxides indicate that $U \cong 5$ eV. This implies that within the models considered here the variations in T_c are mainly due to different values of n in these superconducting materials.

We consider now two special forms of eq. 2:
i) If $f(t/U,n) = g(t/U)h(n)$, then neglecting the volume dependence of U we obtain

$$\frac{d\ln T_c}{d\ln V} = \frac{d\ln t}{d\ln V}\left(2 + \frac{d\ln g}{d\ln(t/U)}\right) \qquad (3)$$

and consequently $d\ln T_c/d\ln V$ is independent of n in contradiction with experimental data. This applies, for example, to the two limiting cases of (eqs. 4.21 and 4.22) considered by Robaszkiewicz et al. (8) in their treatment of the generalized periodic Anderson model with strong local attraction. It applies also to models in which T_c is calculated on the basis of a free Bose gas on a lattice as then $T_c \propto t\, n^{-2/3}$.
ii) If $f(t/U,n) = g(Uh(n)/t)$ then,

$$\frac{d\ln T_c}{d\ln V} = \frac{d\ln t}{d\ln V}\left(2 + \frac{d\ln g}{d\ln(Uh(n)/t)}\right) \qquad (4)$$

and $d\ln T_c/d\ln V$ may strongly be dependent on the band filling. One of the model which leads to an expression of the form indicated here is that of Cyrot (9) for which $h(n) = n$. It is then possible to express $d\ln T_c/d\ln V$ in terms of T_c as shown in Fig. 3. This universal curve

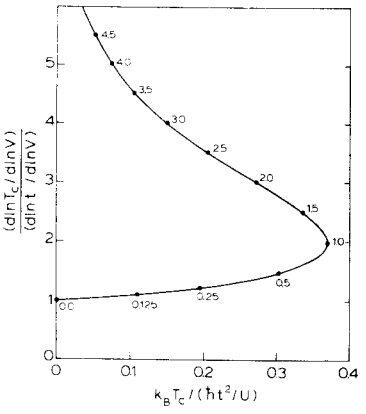

Fig. 3 Prediction of a Hubbard-like model (9). Un/t is indicated at various points

shows that large (and negative, because of $d\ln t/d\ln V \approx -2$) $d\ln T_c/d\ln V$ values are possible for superconductors with low T_c when the concentration of carriers is such that $Un/t \ll 1$.

4. CONCLUSIONS

We have shown that the general trend observed for $d\ln T_c/d\ln V$ may be used to test the validity of theoretical models. In this context it is highly desirable to investigate La-Ba-Cu-O and La-Sr-Cu-O single crystals as these systems have very large volume derivatives of T_c

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