Compressibility of the high- T_c superconductor La_{1.7}Ba_{0.3}CuO_{4-v}

R. Moret and Alan I. Goldman^{*}

Laboratoire de Physique des Solides, Université de Paris-Sud, 91405 Orsay, France

A. Moodenbaugh

Department of Physics, Brookhaven National Laboratory, Upton, New York 11973

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We report on x-ray diffraction measurements of the pressure dependence of the cell parameters of La_{1.7}Ba_{0.3}CuO_{4-y} at room temperature up to 45 kbar. The compressibility $\kappa \approx 5.6 \times 10^{-4}$ kbar⁻¹, and is nearly isotropic above 7 kbar. However, the contraction of the basal plane *a* lattice parameter appears to be negligible at lower pressure, indicating a possible structural change near 7 kbar which may be associated with a previously reported anomaly in the pressure dependence of T_c .

In the high- T_c superconducting oxides of the $La_{1-x}M_{x}CuO_{4-y}$ family (*M* = Ba,Sr,Ca) several studies have shown that T_c strongly increases with pressure. In fact, dT_c/dP is about 1 order of magnitude larger than in the previously studied superconductors. In multiphased samples of nominal composition $La_{1-x}M_xCuO_{4-y}$ (x=0.15 or 0.2), the onset temperature T_c^{onset} increases from 32 K (P = 1 bar) to 40.2 K (P = 13 kbar) at a rate of $dT_c^{\text{onset}}/dP = 0.63 \text{ K/kbar.}^1$ Subsequent measurements of the temperature dependence of the zero resistance temperature T_c^{zero} have yielded $dT_c^{\text{zero}}/dP = 0.12$ K/kbar and $dT_c^{\text{onset}}/dP = 0.31$ K/kbar in La_{1.85}Ba_{0.15}CuO₄.² Similar measurements on the Sr-doped samples have found $dT_c^{\text{zero}}/dP = 0.2$ K/kbar for x = 0.15 (Ref. 3) and $dT_c/dP = 0.295$ K/kbar for x = 0.2 (Ref. 4). In addition, filamentary superconductivity in the pure compound, La_2CuO_4 , has been observed, ^{5,6} with T_c increasing from 37.6 K (1 bar) to 42.4 K (19 kbar) and $dT_c/dP = 0.25$ K/kbar. All of these studies have indicated a continuous pressure dependence of T_c . However, other measurements have revealed an anomaly in dT_c/dP for the Ba-, Sr-, and Ca-doped alloys. Two pressure regions were identified: for $P < P_c$, $dT_c/dP = 0.13$ (Ca), 0.2 (Sr), and 0.1 (Ba) K/kbar, while for $P > P_c$, $dT_c/dP = 0.075$ (Ca), 0.116 (Sr), and 0.04 (Ba) K/kbar. The critical pressure P_c is about 7.3, 4.7, and 6.4 kbar for Ca-, Sr-, and Badoped alloys, respectively.⁷

The unusually large pressure effects are not clearly understood at present. Considering the important role of the Cu-O bonds to current models of superconductivity in these oxides, some knowledge of the compressibility, especially in the basal plane, is useful. In addition, the abovementioned anomaly in dT_c/dP at P_c may point to some structural change⁷ which should be observed in the pressure dependence of the lattice parameters.

The present study was performed on a polycrystalline sample of $La_{1.7}Ba_{0.3}CuO_{4-y}$ prepared by mixing the appropriate quantities of La, Ba, and Cu oxides, pressing the mixture into a pellet, and heating the pellet in air at 1100 °C. Preliminary x-ray measurements showed that 90% of the sample was in the tetragonal K₂NiF₄ phase, and the onset of superconductivity was measured resistively to be

25 K.

The pressure dependence, at room temperature, of the lattice parameters was measured using a diamond-anvil pressure cell with a 4:1 methanol-ethanol solution as a pressure transmitting medium. X-ray powder diffraction data were obtained using Mo $K\alpha$ radiation from a 12 kW rotating anode focused by a bent graphite monochromator. The pressure was determined from the lattice parameters of AgI powder, added to the pressure cell and monitored during the experiment, and its known compressibility.⁸ The cell constants of La_{1.7}Ba_{0.3}CuO_{4-y} were refined from the observed d values of the (101), (004), (103),



FIG. 1. Pressure dependence of the lattice parameters a and c and the unit-cell volume measured at room temperature. The size of the squares corresponds to the estimated experimental error.

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(110), (112), and (114) reflections. No significant change (e.g., new lines) was observed as the pressure was varied.

The cell parameters and volume measured at ambient pressure, 7, 27, and 45 kbar, are plotted in Fig. 1. In spite of the limited number of data points, it appears that the a lattice parameter remains constant up to at least 7 kbar. At higher pressure, there is a linear contraction yielding $(da/a)(1/dP) \approx 2 \times 10^{-4}$ kbar⁻¹. In contrast, no lowpressure plateau is observed for the *c* lattice parameter, which contracts monotonically with (dc/c)(1/dP) $\approx 1.7 \times 10^{-4}$ kbar⁻¹. It then follows that the volume of the tetragonal unit cell shows little compression below 7 kbar, and then decreases at a rate of $\kappa = (dV/V)$ $\times (1/dP) \approx 5.6 \times 10^{-4}$ kbar⁻¹.

The observed anomaly in the pressure dependence of a suggests a possible relation to the anomalous pressure dependence of T_c reported by Shelton, Folherts, Klavins, and Ku⁷ in the La_{1.85} $M_{0.15}$ CuO₄ material. Although our sample contains twice as much Ba, the kink appears at roughly the same critical pressure. This, and the fact that we did not detect any splitting of the reflections over the whole pressure range, indicates that the tetragonal-to-orthorhombic transition cannot be responsible for this effect. This is consistent with the observation of the same anomaly in dT_c/dP for La_{1.85}Ca_{0.15}CuO₄ which is orthorhombic.⁷ In addition, our value for the compressibility is close to that estimated by Shelton *et al.* in their calculation of $\gamma_G \kappa$, the leading-order contribution to $d \ln T_c/dP$.

- *Permanent address: Brookhaven National Laboratory, Upton, NY 11973.
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This then confirms their claim that the higher-order contribution, proportional to the electron-electron interaction parameter g, must have a strong pressure dependence.

Other data on the pressure dependence of the cell parameters in these oxides have been reported by Dietrich *et al.*⁴ and Takahashi *et al.*⁹ for La_{1.8}Sr_{0.2}CuO₄. Our value for κ compares well with theirs and those of other related oxides.¹⁰ However, in contrast to our results, both Refs. 4 and 9 report a smooth decrease in the basal-plane lattice parameter as a function of pressure, although Dietrich *et al.* do note an increase in the compressibility above 20 kbar (this seems to be related to an anomalous decrease in the *c* axis lattice parameter in this case). Clearly, further work is needed to verify the existence of these anomalies, and to relate them to possible structural changes and changes in the electronic properties.

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