Structural transition of $YBa_2Cu_3O_{6.9}$ due to a shock compression up to 270 kbar

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Subjecting the ceramic Y–Ba–Cu–O of the 1-2-3 composition to shock compression ($p = 270$ kbar) produces a ceramic of the same composition which under normal conditions ($p = 0$, $T = 300$ K) has a tetragonal structure with a lattice constant $c = 11.710$ Å and which undergoes a transition to the superconducting state at a temperature $T_{c0} \approx 93$ K.

The ceramics $YBa_2Cu_3O_{7-x}$ are now known to have an orthorhombic lattice or a tetragonal lattice, depending on the heat treatment.[1–4] Ceramics whose structure is orthorhombic are characterized by a crystallographic parameter $c < 11.70$ Å, oxygen deficiency $x < 0.2$, and a superconducting transition temperature of $T_c \approx 90$ K. This

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structure is distinguished by linear Cu–O chains. A tetragonal phase which is devoid of such chains either does not have a superconducting state (when $c > 11.76$ Å) (Refs. 2 and 3) or it undergoes a transition to the superconducting state at lower temperatures, $T_c \approx 50$–60 K (when 11.72 Å $< c < 11.76$ Å) (Refs. 5 and 6).

In the present letter we report the synthesis, by means of a dynamic compression,[7] of the ceramic $YBa_2Cu_3O_{6.9}$ with a tetragonal structure and a superconducting transition temperature $T_{c0} \approx 93$ K.

The original $YBa_2Cu_3O_{6.9}$ samples have an orthorhombic symmetry which is of a single phase, according to x-ray measurements: $a = 3.822$ Å, $b = 3.891$ Å, and $c = 11.672$ Å. These samples are disks 10 mm in diameter and 2.5–4 mm thick. The density of the samples is 4.7 g/cm^3 ($\approx 74\%$ of the crystallographic density of $YBa_2Cu_3O_7$). Measurements of the temperature dependence of the magnetic susceptibility, $\chi(T)$, show that the superconducting transition begins at $T_{c0} \approx 90$ K and that its width is $\leqslant 10$ K in the 10–90% range of variation of χ.

Shock compression of the samples was performed in special cells similar to those described in Refs. 7 and 8. An explosive device of this type is shown schematically in Fig. 1a. This device along with the sample was precooled in liquid nitrogen (the initial temperature of the sample was 90 ± 5 K). A plane detonation wave is formed in

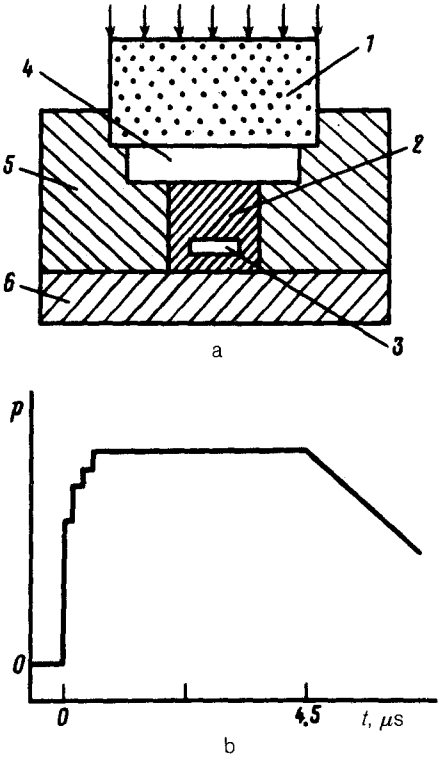

FIG. 1. (a) Schematic diagram of the explosive device; (b) p-t diagram of the sample compression.

charge 1 holding the explosive material. The compression in container 2, which holds the original sample 3, is produced by stopping the dispersing products of the explosion. The air gap which separates the charge from the container provides a constant pressure behind the shock wave front. The size of the container, of the steel can 5, and of the brass lining 6 were chosen in such a way that the maximum fracture strength would be concentrated outside the container that holds the sample. As a result, the assembly surrounding the container was destroyed completely after the experiment, while the container itself remained intact. The original shape of the sample could not be retained in most cases after the shock compression. The sample usually broke up and its further measurements were carried out in the powdered state.

Figure 1b is a plot of the compression of the sample as a function of time. In a time ~ 0.4 μs the sample undergoes multiple compressions by the shock waves to a pressure characteristic of a given explosive device. The maximum pressures reached in various experiments were: 90, 125, 135, 165, 185, 200, 225, 245, and 270 kbar. After holding the compressed and shock-wave-heated sample for 4 or 5 μs, the pressure dropped to atmospheric pressure in several microseconds and the sample's temperature decreased by about half.

The crystal structures of compressed samples were studied at room temperature in a Debye chamber and x-ray diffractometer (Cu $K\alpha$ radiation, scanned in the range $10° < 2\theta < 70°$). The stressed state of the ceramic resulting from shock compression caused all diffraction peaks to broaden, but the ratio of the widths at half-maximum of the various peaks changed only slightly. For the 113 and 020 lines, for example, this ratio ranged from 0.6 to 0.8 over the entire pressure range. The diffraction patterns had no additional lines, except those corresponding to the 1-2-3 phase of the ceramic.

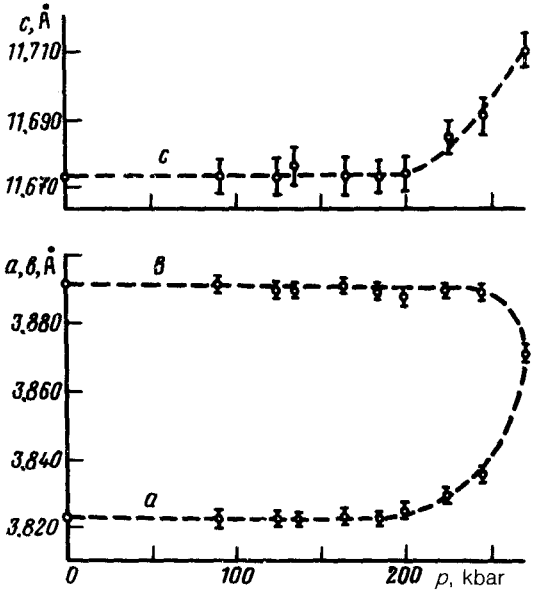

FIG. 2. Dependence of the lattice constants a, b, and c, on the pressure p.

The lattice constants a, b, and c are plotted in Fig. 2 as a function of the pressure p. In the pressure region $200 \leqslant p \leqslant 270$ kbar we see that the lattice symmetry rises from orthorhombic to tetragonal. It is of particular interest that the structural transition is accompanied by only a slight change of the lattice constant c; at $p = 270$ kbar we have $c = 11.710 \pm 0.005$ Å.

The structural changes may be caused not only by compression but also by a sharp variation in temperature which is usually high in the case of shock compression of porous samples.[9]

A correlation has been established between the concentration of oxygen in $YBa_2Cu_3O_{7-x}$ and the lattice constant c. Analysis of the experimental data carried out in Refs. 10 and 11 has shown that c depends linearly on x: $x = 5.16$–60.08. If this ratio is valid in our case, the ceramic with a tetragonal structure, obtained as a result of a shock compression at $p = 270$ kbar, would have the approximate composition $YBa_2Cu_3O_{6.7}$ with a sufficient amount of oxygen.

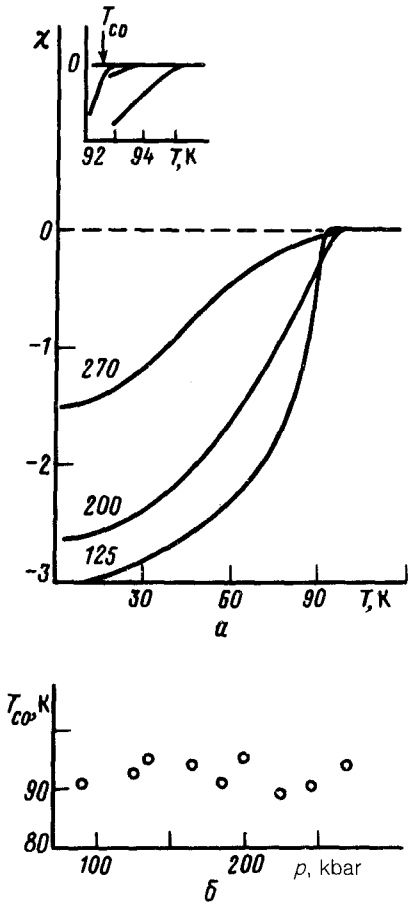

FIG. 3. (a) Typical $\chi(T)$ curves for powder samples obtained as a result of shock compression at the pressures 125, 200, and 270 kbar (shown to the left of the curves); (b) temperature of the onset of the transition, T_{c0}, versus the pressure.

Figure 3a shows plots of χ vs T (in arbitrary units) obtained under the same conditions (the frequency of the alternating field—80 Hz, the amplitude—1 Oe; the sensitivity of the measuring circuit was constant) for powdered $YBa_2Cu_3O_{7-x}$ samples synthesized at pressures of 125, 200, and 270 kbar. The reversible $\chi(T)$ curves were reproduced many times. The superconducting transition of a shock-compressed ceramic is markedly broader than that of the original sample. With an increase in pressure, the slope of the diamagnetic part of the $\chi(T)$ curve, moreover, becomes less steep and at $p = 270$ kbar the $\chi(T)$ curve has an additional inflection point near 60 K. The initial temperature of the transition, T_{c0} whose plot is shown in the inset in Fig. 3a, nonetheless changes only slightly in the case of all test samples: $89 < T_{c0} < 95$ K (Fig. 3b).

A shock compression of the original $YBa_2Cu_3O_{6.9}$ ceramic at pressures $p > 200$ kbar thus produces a tetragonal phase with a smaller than usual lattice constant c and with apparently only a small loss of oxygen. The ceramic obtained at $p = 270$ kbar retains its superconducting properties ($T_{c0} \approx 93$ K), suggesting that the presence of the Cu–O chains in the high-T_c superconductivity mechanism does not play a critical role.

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