Thermal expansion of $YBa_2Cu_3O_7$ single crystal

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The thermal expansion of a $YBa_2Cu_3O_7$ single crystal has been studied by x-ray diffraction at temperatures from 4 K to 180 K. It is stressed that the thermal expansion along the *b* direction is anomalous.

In this letter we are reporting a study of the thermal expansion of a $YBa_2Cu_3O_7$ single crystal by x-ray diffraction over the temperature range from 4 K to 180 K. The experimental results cannot be interpreted completely unambiguously, although they evidently indicate that the b direction (parallel to the Cu–O chains) plays a special role in the $YBa_2Cu_3O_7$ crystal.

The experiments were carried out with a three-crystal spectrometer (developed at the Institute of Crystallography, Academy of Sciences of the USSR), which works in a two-beam arrangement with an analyzer—a high-quality Si (220) crystal—serving as a standard. The radiation source was a molybdenum tube (40 kV, 30 mA).

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The $YBa_2Cu_3O_7$ single crystal (with dimensions of $1\times1\times0.03$ mm) selected for this study was grown by spontaneous crystallization from a nonstoichiometric melt[1] and then annealed in oxygen. Examination of the crystal under a microscope revealed a pronounced domain structure, characteristic of twinning along the [110] direction. The initial rocking curve of the crystal had a half-width $\sigma = 1.2'$. Measurements of the ac magnetic susceptibility showed that this crystal has a fairly sharp superconducting transition ($\Delta T < 1$ K) at $\simeq 90$ K.

In the course of the measurements, the crystal was cemented to a beryllium plate, which was in turn attached to a copper block in the vacuum chamber of a helium cryostat. The sample temperature was regulated within 0.01 K. The temperature was measured by a platinum resistance thermometer.

The first measurements showed that this crystal consists of two blocks, with slightly different lattice constants [$a_1 = 3.8098(2)$, $b_1 = 3.8808(2)$; $a_2 = 3.8120(2)$, $b_2 = 3.8824(2)$; $T = 4.2$ K (Fig. 1)]. After a few cooling–heating cycles, however, it was found that the rocking curve of the sample and the diffraction curves were becoming progressively narrower, and the peaks progressively smaller. The splitting of the diffraction peaks subsequently became undetectable, and the half-width of the rocking curve stabilized at about $\sigma = 0.8'$. The lattice constants of this crystal assumed the values $a = 3.8085(2)$, $b = 3.8811(2)$, $c = 11.6424(2)$.

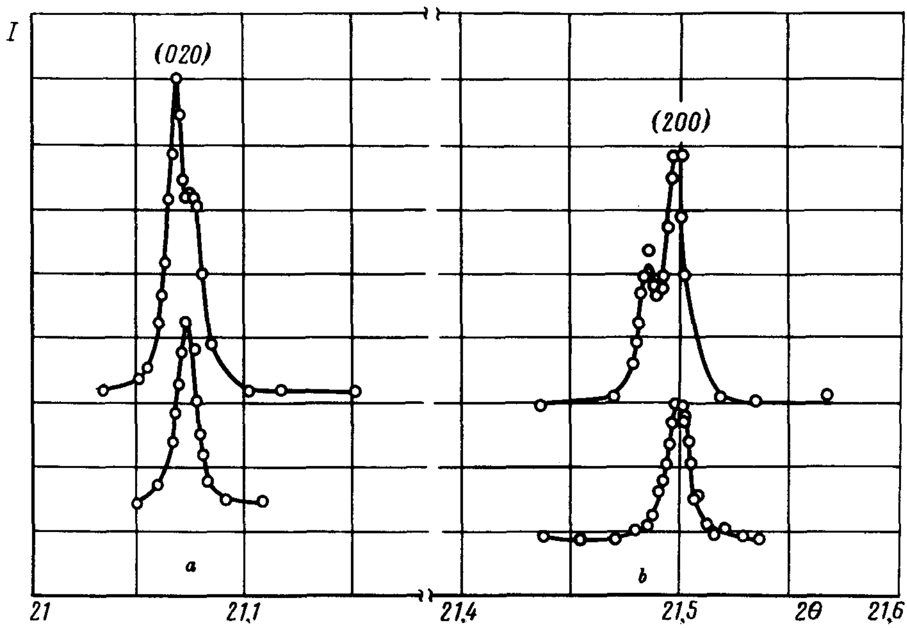

FIG. 1. Diffraction peaks for a $YBa_2Cu_3O_x$ single crystal at $T = 4$ K. *a*—First cooling; *b*—after several cooling cycles.

In summary, and in contradiction of Ref. 2, we found it possible to study a crystal of satisfactory quality whose diffraction peaks can be described by a single Lorentz function.

In the subsequent study of the thermal expansion of the $YBa_2Cu_3O_7$ crystal, we studied the temperature dependence of the angular positions of the (200), (020), and (006) diffraction peaks. The behavior of each peak was studied in a separate experiment in which the temperature was varied. The error in the determination of each of the lattice constants was on the order of 2×10^{-4} Å.

The experimental results are shown in Fig. 2. The thermal expansion of the crystal is described by an expression of the following type[3] along each of the directions *a*, *b*, *c*:

$$l_i = l_{i,0} + A_i f_E(\Theta_i/T), \tag{1}$$

where $i = a,b,c$; $l_{i,0}, A_i, \Theta_i$ are constants; and f_E is the Einstein function.

A fit of the data revealed that the effective Einstein temperature for the *b* direction was far higher than the corresponding temperatures for the *a* and *c* directions; the two latter temperatures turned out to be very nearly the same: $\Theta_a^E = 195(14)$, $\Theta_b^E = 304(22)$, $\Theta_c^E = 187(5)$.

The curves of the expansion of the $YBa_2Cu_3O_7$ crystal are thus fairly smooth, without any structural features at the transition point. The expansion curve shown here seemed to be an excellent illustration of this behavior (Fig. 3). Nevertheless, the

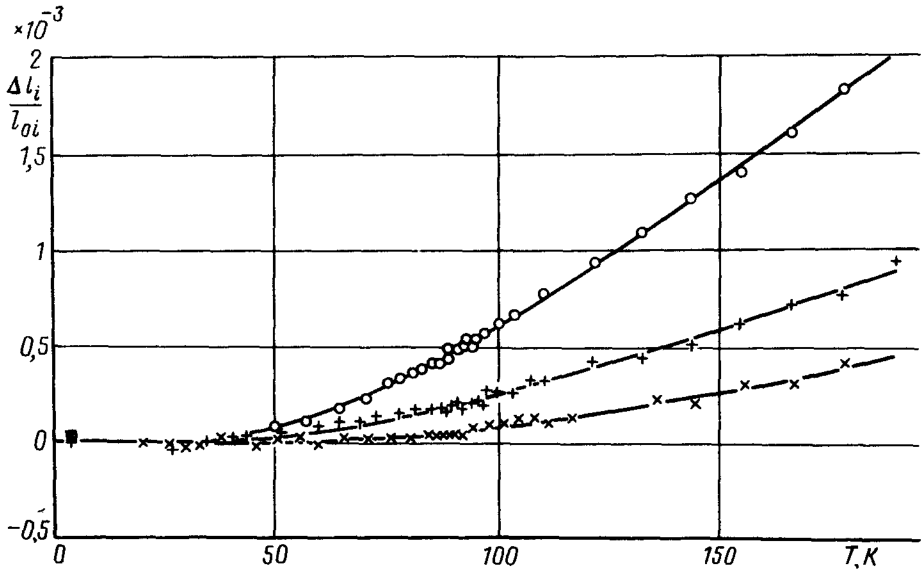

FIG. 2. Temperature dependence of the lattice constants of $YBa_2Cu_3O_x$, in the coordinates $\Delta l_i/l_{0i} - T$.

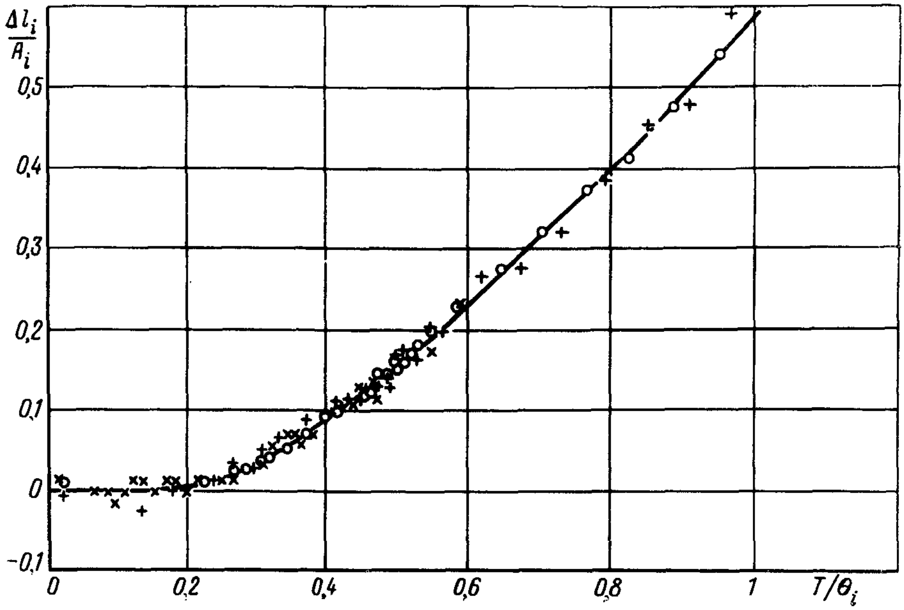

FIG. 3. Thermal expansion of a $YBa_2Cu_3O_x$ single crystal, in the coordinates $(l_{iT} - l_{0i}/A_i) - T/\Theta^E$ [see Eq. (1)].

exceedingly high characteristic frequency corresponding to the thermal vibration along the b direction requires some explanation, especially since the linear compressibilities of the $YBa_2Cu_3O_7$ crystal along the a and b directions are very nearly the same.[4] One possible explanation of this situation might thus be that a specific frequency dependence and a specific coordinate dependence of the Grüneisen coefficient γ_{ik} suppress the contribution of low-frequency phonons to the thermal expansion along the b direction. What we are actually dealing with here is the existence of "soft" low-frequency modes in the thermal vibration spectrum of $YBa_2Cu_3O_7$.

On the other hand, the poorly defined inflection point on the temperature dependence of the orthorhombic parameter $2(b-a)/(b+a)$ is interesting. This point is localized near the superconducting transition ($\simeq 90$ K; Ref. 4). It can be seen from Fig. 4 that this structural feature is associated with a pronounced maximum on the curve of $(\alpha_b - \alpha_a)(T)$, where α is the thermal expansion coefficient calculated from expressions (1). This circumstance makes it equally plausible to suggest that an anomalously high value of the characteristic temperature Θ_E is being simulated by a sharp decrease in the thermal expansion coefficient α_0 upon the transition to the superconducting state.

To estimate the amplitude of the expected jump, $\Delta\alpha_b$, we can approximate the high-temperature part of the experimental data on $b(T)$ at $T > 90$ K by an expression like (1), but with a fixed temperature $\Theta^E = 195$, equal to the temperature found through an approximation of the thermal expansion along the a direction. When we

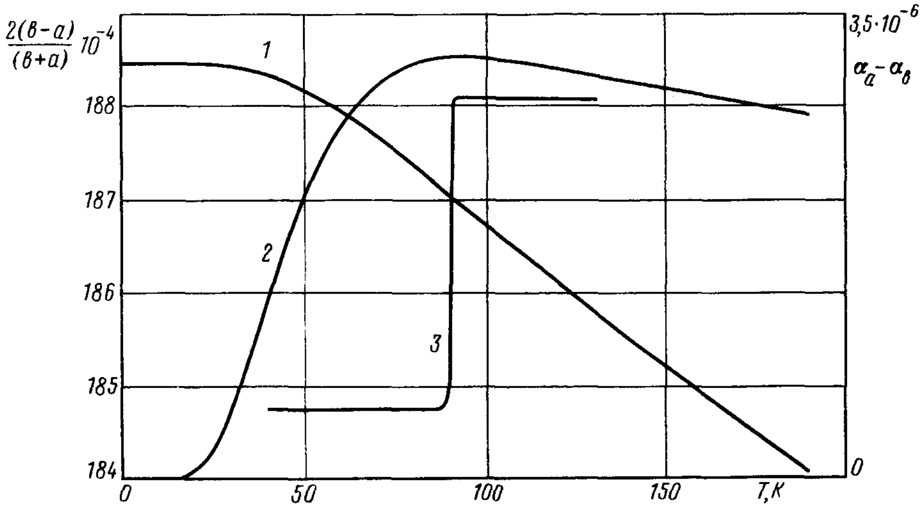

FIG. 4. *1*—The orthorhombic parameter $2(b-a)/(b+a)$; *2*—the difference in thermal expansion coefficients $\alpha_b-\alpha_a$; *3*—*the jump in the magnetic susceptibility at the point of the superconducting transition for* the $YBa_2Cu_3O_7$ single crystal studied. Approximations (1) were used in the calculation of the orthorhombic parameter and the thermal expansion coefficients.

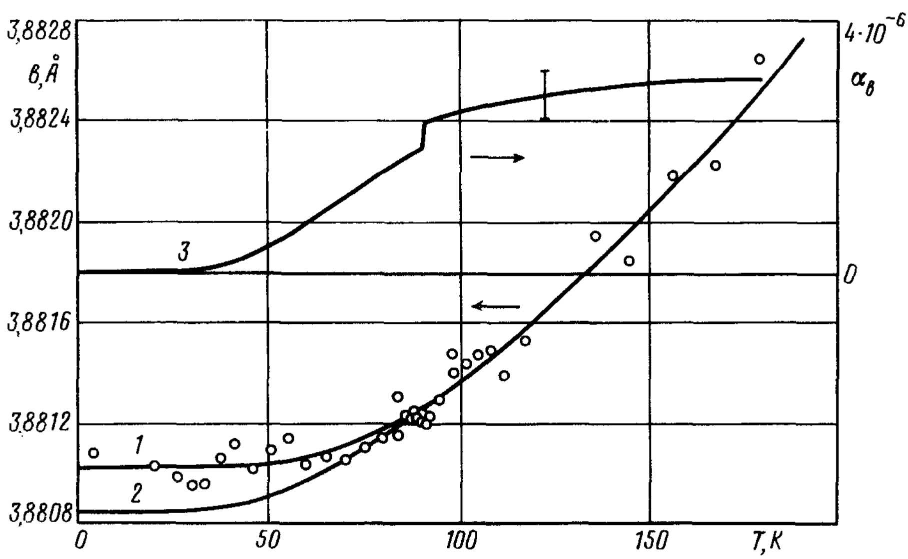

FIG. 5. Diagram used in calculating the jump in the thermal expansion coefficient $\alpha_b=(1/b)(db/dT)$ at the point of the phase transition. O—Experimental points; *1*—approximating curve of the type in (1) calculated with the help of all the experimental points (Θ_b^E is an adjustable parameter); *2*—approximating curve of the type in (1) calculated from the experimental points at $T>90$ K (Θ^E is assumed to be $\Theta_a^E=195$ K); *3*—temperature dependence of the thermal expansion coefficient $\alpha_b=(1/b)(db/dT)$. The calculation was based on the data of two approximations. The calculation error is shown in the figure.

then compare the coefficients α_b at $T = 90$ K found by the two approximations, we can estimate the possible jump $\Delta\alpha_b$. The corresponding construction is shown in Fig. 5; the jump $\Delta\alpha_b$ turns out to be 0.5×10^{-6} grad^{-1}.

We of course cannot rule out from our discussion of the experimental results the existence of jumps in the thermal expansion in the other directions in the crystal, but the amplitude of such jumps should be substantially smaller than $\Delta\alpha_b$.

The sign found for $\Delta\alpha_b$ as a result of this analysis points unambiguously to a negative slope of the superconducting transition curve dT_c/dp for $YBa_2Cu_3O_7$. Although this conclusion agrees with the results of Ref. 5, precise measurements of dT_c/dp could serve as a critical test of the last of these suggested interpretations of the experimental results.

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