Thermal expansion and elastic properties of the high-temperature superconductors (Y, Ho)$Ba_2Cu_3O_7$

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Parameters of the crystal structure, the thermal expansion, and the Young's modulus of superconducting ceramics based on yttrium and holmium have been measured at various temperatures. Anomalies observed in the temperature dependence of these characteristics are linked with an ordering of oxygen vacancies.

Information of importance for identifying the mechanism for the superconductivity in the new class of high-temperature superconducting ceramics $MBa_2Cu_3O_7$ ($M = Y$ or a rare-earth ion) is how the superconducting and structural characteristics are interrelated. In this letter we report both direct low-temperature x-ray-diffraction studies of the crystal structure of superconducting ceramics based on Y and Ho and measurements of their structure-sensitive characteristics: the thermal expansion $\Delta L/L$, the Young's modulus E, and the internal friction Q^{-1}.

In the measurements we used samples synthesized by a ceramic technique[1,2] which are of a single phase (the 1-2-3 phase), according to x-ray measurements. The temperature of the superconducting transition, T_c, was 93–95 K, and the width of the transition was $\Delta T_c \lesssim 2$ K. The linear expansion was measured by a strain-gauge method,[3] while the Young's modulus and the internal friction were measured with the help of a composite vibrator at a frequency of 200 kHz (Ref. 4). For the x-ray measurements we used a Geigerflex diffractometer (manufactured in Japan). The lattice constant c was determined from the isolated (0, 0, 11) reflection.

Figure 1 shows the temperature dependence of the thermal expansion and of the relative Young's modulus $\Delta E/E_0$, where $\Delta E = E(T) - E_0$, $E_0 = E$ (130 K), of yttrium- and holmium-based ceramics (a and b).

It can be seen from Fig. 1a that at $T \sim T_c = 93$ K the curve of $\Delta L/L(T)$ for $YBa_2Cu_3O_7$ has a clearly defined anomaly: a local decrease (over an interval ~ 10 K) in the temperature coefficient of linear expansion, α, by an amount $\Delta\alpha \sim 6 \times 10^{-6}$ K^{-1} [$\alpha(90\text{ K}) \approx \alpha(100\text{ K}) \approx 8 \times 10^{-6}$ K^{-1}]. A similar anomaly in $\Delta L/L$ at $T \gtrsim T_c$ was observed in the $HoBa_2Cu_3O_7$ samples (Fig. 1b). An estimate of the expected jump in α at the superconducting transition on the basis of thermodynamic considerations, specifically, from the formula $\Delta\alpha = (1/4\pi)(\partial T_c/\partial p)(\partial H_c/\partial p) = \alpha_n - \alpha_s$, yields the value $\Delta\alpha \sim 1.5 \times 10^{-7}$ K^{-1} for $YBa_2Cu_3O_7$ (for this estimate we used the values $\partial T_c/\partial p = 0.45$ K/GPa (Ref. 5) and $\partial H_c/\partial T \sim 400$ Oe/K (Ref. 6). This value is

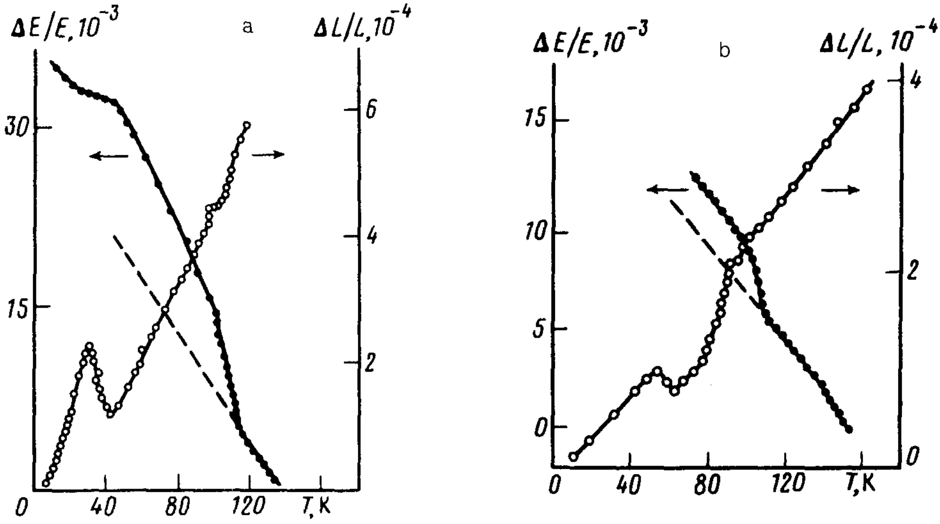

FIG. 1. Temperature dependence of the thermal expansion $\Delta L/L$ and the Young's modulus $\Delta E/E$. a—$YBa_2Cu_3O_7$; b—$HoBa_2Cu_3O_7$.

considerably smaller than the magnitude of the observed anomaly.

On the temperature dependence of $\Delta E/E_0$, this structural feature corresponds to an interval of an anomalous increase in the Young's modulus $\Delta E/E_0 \sim (2\text{–}5)\times 10^{-3}$. In the same temperature region (90–120 K) we also observe a maximum of the internal friction Q^{-1} (Fig. 2). In the low-temperature region (at 40 K for $YBa_2Cu_3O_7$ and

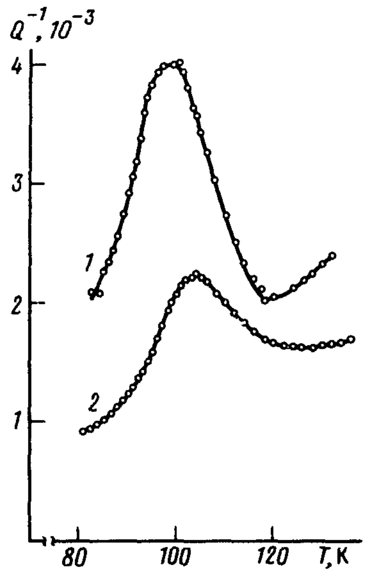

FIG. 2. Temperature dependence of the coefficient of internal friction, Q^{-1}. 1—$YBa_2Cu_3O_7$; 2—$HoBa_2Cu_3O_7$.

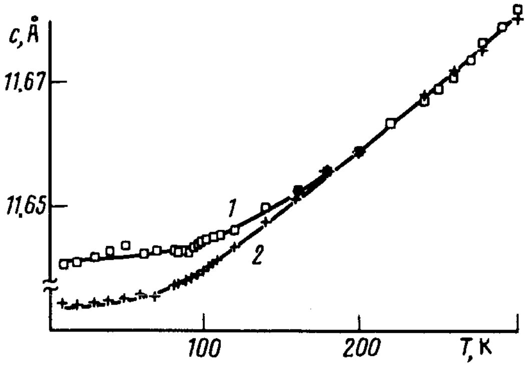

FIG. 3. Temperature dependence of the lattice constant c of $YBa_2Cu_3O_7$. 1—Measurements in an oxygen atmosphere; 2—measurements in a vacuum, at $p \sim 10^{-2}$ torr.

at 60 K for $HoBa_2Cu_3O_7$), there is an even sharper anomaly in the thermal expansion, which is also manifested as a change in the slope of the temperature dependence of $\Delta E / E_0$. The magnitudes of all the observed anomalies vary from sample to sample and are smallest in the case of $GdBa_2Cu_3O_7$.

Low-temperature x-ray-structural studies carried out with powdered $YBa_2Cu_3O_7$ samples showed that these anomalies are also manifested in the temperature dependence of the lattice constant, $c(T)$ (curve 1 in Fig. 3). It was found, however, that this dependence is strongly influenced by the experimental conditions. In the case of cooling in an O_2 atmosphere (curve 1), the behavior $c(T)$ is approximately that described by the Debye law with a Debye temperature $\Theta_1 = 560$ K. A prolonged hold and cooling in a vacuum of 10^{-2} Torr (which apparently results in a reduction in the amount of oxygen in the sample) results in the disappearance of the low-temperature anomalies; over the entire interval studied, the $c(T)$ curve can be described by a Debye law with a considerably lower Debye temperature, $\Theta_2 = 310$ K. These results indicate that the oxygen content in the sample has a strong influence on the lattice dynamics.

The anomalies which we observed in the thermal expansion and elastic characteristics in this study (at least in the interval 90–110 K) are, in our opinion, related to an ordering of oxygen vacancies and the formation of continuous linear Cu-O chains along which the material conducts. At $T \lesssim 110$ K, the oxygen apparently leaves positions which do not correspond to the ordered structure $YBa_2Cu_3O_7$ and fills vacancies along the Cu-O chains. The "binding" of the initially ruptured pieces of the chains may lead to the formation of a more intense effective phonon spectrum $\alpha^2 F(\omega)$ and to an intensification of the electron-phonon interaction for electrons moving along these chains. An accentuation of the structure of the phonon spectrum upon a lowering of the temperature was observed for a lanthanum ceramic by Renker *et al.*, although in that case the ordering of the oxygen occurs not in chains but in Cu-O planes. The ordering process may be the reason for the observed anomalies in the thermal, elastic, and structural characteristics. It may also lead to a strong electron-phonon interaction which causes the high-temperature superconductivity.

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