Anomalous behavior of the structural parameters of the ceramic $YBa_2Cu_3O_7$ near the superconducting transition

A. I. Golovashkin, O. M. Ivanenko, G. I. Leĭtus, K. V. Mitsen, O. G. Karpinskiĭ, and V. F. Shamraĭ
P. N. Lebedev Physics Institute, Academy of Sciences of the USSR

(Submitted 15 July 1987)
Pis'ma Zh. Eksp. Teor. Fiz. **46**, No. 8, 325–327 (25 October 1987)

Low-temperature x-ray-structural analysis of single-phase samples of the superconducting ceramic $YBa_2Cu_3O_7$ was carried out. The temperature dependence of the lattice constants and of the unit cell volume was found to behave anomalously near the superconducting transition. This anomaly is linked with the ordering of the oxygen vacancies.

The superconducting ceramic $YBa_2Cu_3O_7$ exhibits an anomalous behavior in the sound velocity, elastic modulus, and linear expansion coefficient near the superconducting transition.[1] This behavior suggests, in particular, that there is a lattice deformation in this temperature interval. To verify this assumption, we carried out a low-temperature x-ray structural analysis of some samples of the superconducting ceramic $YBa_2Cu_3O_7$. The samples were prepared using the technology described in Ref. 2. Special efforts were taken to insure sample homogeneity by controlling the width of the x-ray diffraction peaks and the sharpness of the diamagnetic transition. The temperature of the transition to the superconducting state, T_c, measured from the change in the resistance of the samples, was 93 K for a width $\Delta T_c^R \approx 1$ K. The width of the superconducting transition, measured from the susceptibility in a 0.5-Oe field, was $\Delta T_c^\chi \sim 2$ K. Below 89 K the samples were 100% diamagnetic.

The low-temperature x-ray studies were carried out with the DRON-2 diffractometer (the iron $K\alpha$ line) using the powder method. The lattice constants were determined by analyzing the data on 23 "pure" reflections using the method of least squares. The measurements were carried out at temperatures between 77 K and 300 K.

Figure 1 shows the temperature dependences of the orthorhombic lattice constants a, b, and c. The measurement results were obtained by slowly warming the sample which was initially cooled to 77 K. The results of two series of measurements are given. We see from the figure that the lattice constants begin to change markedly as the temperature of the sample approaches T_c and that they return to approximately the original values immediately before the superconducting transition. The maximum deviation of the lattice constants a and c at the minima is $\sim 0.2\%$ and that of the lattice constant b is $\sim 0.1\%$. The deviations are much greater than the measurement error ($\sim 0.02\%$). The temperature interval of the anomalous dependence of the structural parameters corresponds to the region where the deviation from the linear behavior of the temperature dependence of the sample's resistance occurs and also to the

 0021-3640/87/200410-03$01.00

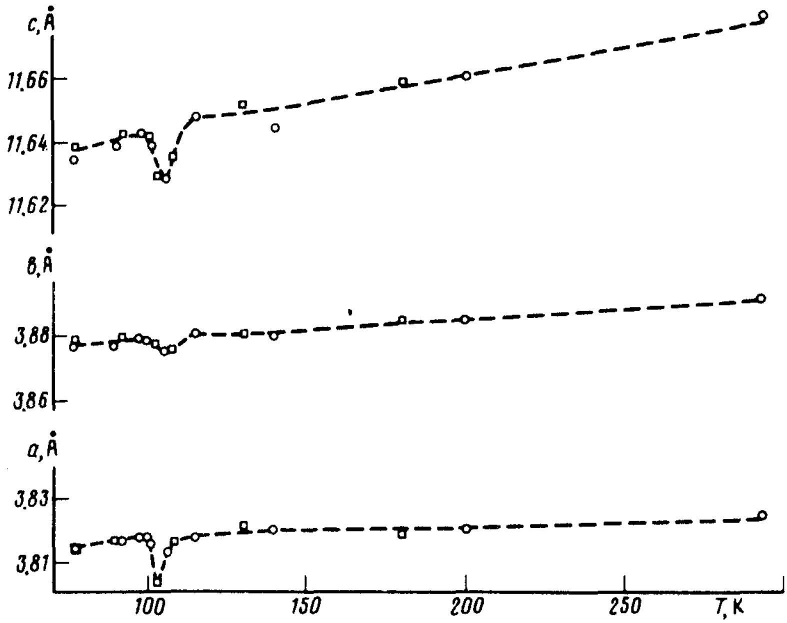

FIG. 1. Temperature dependences of the orthorhombic lattice constants *a*, *b*, and *c* of the ceramic $YBa_2Cu_3O_7$.

region where the temperature dependence of the ultrasound velocity plateaus.[1]

The results in Fig. 1 were obtained after an exposure of about 1 h at each point. Figure 2 shows the temperature dependences of the structural parameters obtained by thermal cycling in the region of the observed anomaly and after an exposure of 20 min

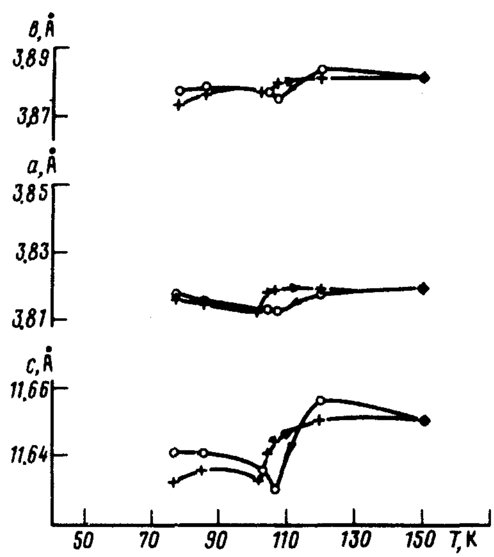

FIG. 2. Temperature dependences of the lattice constants *a*, *b*, and *c* obtained as a result of thermal cycling.

at each point. The arrows indicate the direction of the temperature change. In addition to the distortion of the original dependences, we see a hysteresis due to the thermal cycling. In particular, the lattice parameter c first increases by about 0.01 Å after the sample is returned to its original temperature of 77 K, and then decreases to the original value in several hours.

The peculiar behavior of the structural parameters suggests the presence of some sort of slow, diffusion-type structural relaxation which occurs in the temperature interval preceding the superconducting transition and which may stem from the ordering of oxygen vacancies at these temperatures. The oxygen sublattice, which is assumed to be "soft" in this case, may be responsible for the strong electron-electron interaction that accounts for the superconductivity.

Another possible distortion of the temperature dependence of the structural parameters, which is related to the formation of ice in the pores of the ceramic samples, should, however, be pointed out. The observed anomalous contraction in this case could occur in a certain sequence of the phase transitions during the thermal expansion between the modifications of ice of various densities. Such a sequence of the transitions cannot, however, be found from the known ice modifications.[3] Furthermore, no such anomaly was observed in a lanthanum ceramic with the same porosity, making it extremely unlikely that ice formation can distort the temperature dependence of the structural parameters. Similar measurements using single-crystal samples will enable us to draw a final conclusion.

[1]A. I. Golovashkin, V. A. Danilov, O. M. Ivanenko, K. V. Mitsen, and I. I. Perepechko, Pis'ma Zh. Eksp. Teor. Fiz. **46**, 273 (1987) [JETP Lett. **46**, No. 7 (1987)].
[2]M. R. Wu, J. R. Ashburn, C. J. Torng, P. H. Hor, R. L. Meng, L. Gao, J. Huang, Y. Q. Wang, and C. W. Chu, Phys. Rev. Lett. **58**, 908 (1987).
[3]E. R. Paunder, Physics of Ice, Mir, Moscow, 1967.

Translated by S. J. Amoretty