Low-temperature x-ray diffraction of the Y1Ba2Cu3O9−x oxide ceramic superconductor

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Low-temperature x-ray diffraction of the $Y_1Ba_2Cu_3O_{9-x}$ oxide ceramic superconductor

Hua-qing Yin, Yi-mei Gao, Jia-ju Du, Ben-pei Chen, Jian-yi Jiang, and Xiang Wang
Institute of Solid State Physics, Academia Sinica, Hefei, People's Republic of China

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The change of the lattice parameter with temperature (82–320 K) of the single phase $Y_1Ba_2Cu_3O_{9-x}$ superconductor has been investigated by x-ray diffractometer. The experimental result shows that there exist two abrupt changes of lattice parameter at about 250 and 125 K separately in the curve of the lattice parameter versus temperature. But no change of structure symmetry was observed as shown by x-ray diffraction. The abrupt change of lattice parameter at about 250 and 125 K may be associated to the position adjusting of oxygen atoms in oxide ceramic.

Since the La-Ba-Cu-O system oxide ceramic superconductor was observed by Bednorz and Müller,[1] great progress has been taken both on the theory and experiment. But some of the materials remain to be studied in detail. Many of us are interested in the structure of the oxide ceramic superconductor. To get more knowledge about this kind of material, many experimental methods are used to study its structure features. The results of x-ray and neutron diffraction showed that the $Y_1Ba_2Cu_3O_{9-x}$ crystal has a distorted perovskite structure.[2,3] In our early paper[4,5] we reported that three internal friction peaks and anomalies of Young's modulus were observed and that the peak at about 200 K may be asssociated with the change of the microscopic structure. In this letter the $Y_1Ba_2Cu_3O_{9-x}$ superconductor is investigated by means of a low-temperature (82–320 K) x-ray diffractometer.

The samples used in this study were prepared from mixtures of high-purity Y_2O_3, $BaCO_3$, and CuO powder by a standard ceramic sintering process. Single phase polycrystalline structure was obtained as shown by the x-ray diffraction result. The superconductivity transition temperature was measured to be 90 K.

The TTK x-ray low-temperature vacuum camera of a Philips PW1700 x-ray diffractometer was used to precisely measure the lattice parameter in low temperature (82–320 K). The [006] lattice plane diffraction peak was measured with a scan rate 0.01 deg/s. The sampling interval is 4 s.

The temperature relation of lattice parameter c is shown in Fig. 1. The sample was cooled to 80 K, then was measured with heating temperature step by step. At about 250 and 125 K an abrupt change in the lattice parameter was observed. The [006] lattice plane diffraction peaks for different temperature were given in Fig. 2. A shift of the diffraction peak was observed, but no remarkable change in the peak shape for different temperatures. To give detailed description for the structural change, diffraction scans from 20° to 70° at 250 and 300 K were performed as shown in Fig. 3. Comparing the 250 to the 125 K diffraction patterns, we did not observe any changes in the crystalline symmetry.

From the observations of high-resolution electron microscopy and neutron diffraction study, the structure of $Y_1Ba_2Cu_3O_{9-x}$ superconductor is seen to be an oxygen vacancy distorted perovskite structure. There is also oxygen vacancy on the basal plane of the $Y_1Ba_2Cu_3O_{9-x}$ crystalline unit. The fact that no remarkable structural symmetry transition occurs at 250 K illustrates that the abrupt change of lattice parameter at about 250 K is not due to structural phase transition, but may be associated with the position adjusting of oxygen atoms. In other experiments such as internal friction[4,5] and Raman spectra,[6] an anomalous phenomenon of structure was observed. One possible explana-

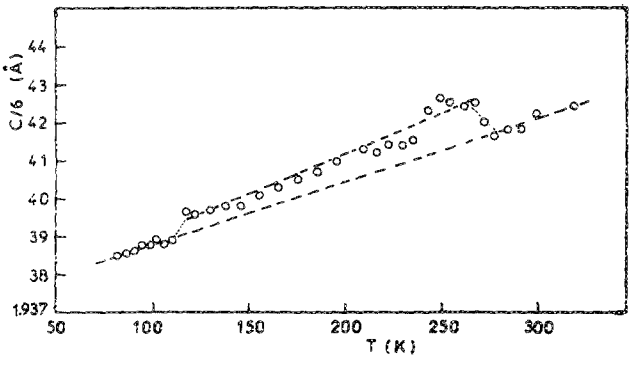

FIG. 1. Relation curve of lattice parameter and temperature.

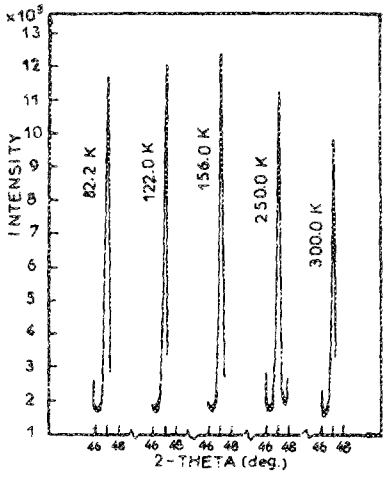

FIG. 2. [006] lattice plane diffraction patterns at different temperatures.

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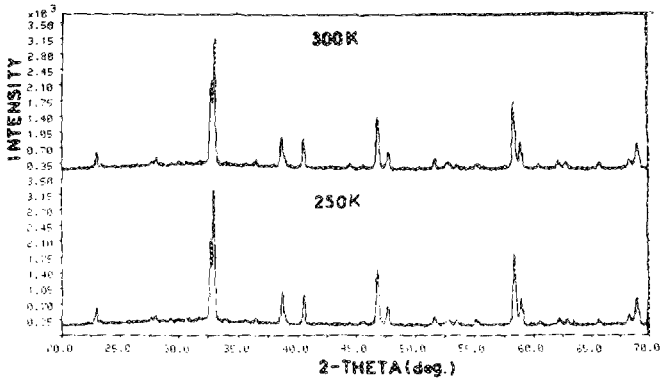

FIG. 3. X-ray diffraction patterns at 300 and 250 K. Cu $K\alpha$ radiation, 40 kV tube voltage, 30 mA tube current are used.

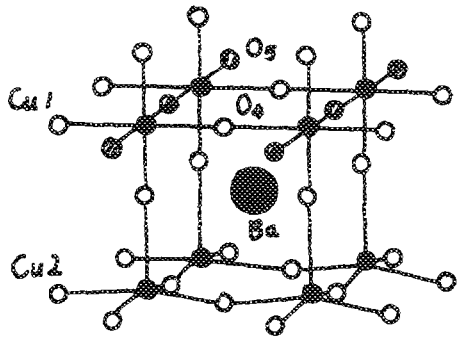

FIG. 4. Schematic representation of crystalline unit basal plane.

tion is that the abrupt change of lattice parameter at about 250 K is associated with the oxygen atoms jumping from an O_4 site to an O_5 site (see Fig. 4). Because the lattice parameter a is not equal to b, the change of orientation of the Cu-O chain must cause the change of length in the Cu-O band along the c axis. To confirm this explanation, other experiments will be done.

In Fig. 1, the expansive rates along the c axis at below 125 K and above 250 K are equal, while between 125 and 250 K the lattice expansion along the c axis is with another expansive rate. Thus a suggestion should be made that an abrupt change of the c value at about 125 K is the converse process at 250 K.

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