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ScienceDirect
Solid State Communications 145 (2008) 246–249
solid state communications
www.elsevier.com/locate/ssc

Spontaneous strain in high-temperature superconductor $La_{1.85}Sr_{0.15}CuO_4$

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Received 1 July 2007; received in revised form 13 October 2007; accepted 18 November 2007 by S. Miyashita
Available online 23 November 2007

Abstract

The lattice parameters of $La_{1.85}Sr_{0.15}CuO_4$ were measured by an x-ray Rietveld method between 15 K and room temperature. A change in a lattice parameter could be detected at superconducting phase transition. It is pointed out, for the first time, that the change can be attributed to a spontaneous strain in the superconducting phase caused by coupling between a superconducting order parameter and the strain.

PACS: 74.72.Dn; 60; 61.05.cp

Keywords: A. High-T_c superconductors; C. Crystal structure and symmetry; D. Phase transitions

1. Introduction

Structural changes in high-temperature superconductors have been studied extensively since the discovery of superconducting phase transition in $La_{2-x}Sr_xCuO_4$ using high-resolution diffractometers. Nevertheless, no significant anomalies could be detected in connection with the superconducting phase transition. Recently, an accurate lattice parameter measurement has been carried out on orthorhombic $YBa_2Cu_3O_{6.5}$ with a superconducting transition temperature T_c of 55 K by high-angle double-crystal x-ray diffractometry: The change in orthorhombicity $2(b-a)/(a+b) = \tan^{-1}(b/a) - \pi/4$ at T_c could be clearly detected [1]. The introduction of a new critical exponent was considered necessary for explaining the difference between the observed orthorhombicity and that extrapolated from the normal state. An anomaly of the lattice parameter a of hexagonal MgB_2 was clearly observed below its superconducting transition temperature $T_c = 39$ K by high-resolution pulse neutron powder diffraction [2]. This result was analysed by introducing two Einstein temperatures, 222 K and 69 K, and two Grüneisen parameters, 1.33 and −0.304. The anomaly of the lattice parameter a of MgB_2 was found to be independent of the onset of superconductivity.

Spontaneous strain is typically produced as a secondary order parameter through the coupling between the strain e and the primary order parameter Q that is an atomic shift in structural phase transitions. The free energy $G(Q,T)$ near the transition temperature T_c can be written in its simplest form as follows using a Landau potential:

$$G(Q,T) = G_0(T) + \frac{1}{2}A(T-T_c)Q^2 + \frac{1}{4}BQ^4 + \frac{1}{2}Ce^2 - DeQ^2,$$

where A, B, C and D are temperature T-independent positive constants. From the equilibrium condition for the strain, we can obtain the relation $e = (D/C)Q^2$. The primary-order parameter Q is zero above T_c, whereas Q is nonzero below T_c. The spontaneous strain is defined as follows by the low-temperature phase lattice parameter a_{LT} and high-temperature phase lattice parameter a_{HT} when extrapolated to the same temperature [3]: $e = (a_{LT} - a_{HT})/a_{HT}$. In the case of tetragonal–orthorhombic structural phase transition, the orthorhombicity $2(b-a)/(a+b)$ is twice the spontaneous strain in the ab-plane, because the lattice parameter of an average structure (i.e. a hypothetical tetragonal structure at a low temperature) is $(a+b)/2 \approx (ab)^{1/2}$ as a first approximation [3]. We have been studying the phenomenological relations of order parameters in the antiferroelectric phase transitions of the perovskites $PbZrO_3$ and $PbHfO_3$ by

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0038-1098/$ - see front matter © 2007 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ssc.2007.11.024

X-ray and neutron diffraction analyses [4,5]: The spontaneous strain perpendicular to the plane in which an antiferroelectric order parameter appears could be explained well by conventional coupling. The strain in the plane, however, showed a complex dependence on temperature, which is difficult to explain in terms of the coupling.

If the spontaneous strain in high-temperature superconductors is caused by the same mechanism as that in structural phase transitions, the strain perpendicular to the CuO_2 plane is expected to show a temperature dependence proportional to the square of a primary order parameter, which is a superconducting gap, because a gap appears in the CuO_2 plane. The lattice parameter c of YBCO changes considerably with decreasing temperature above T_c, which prevents drawing a definite conclusion. The saturation of the lattice parameter above T_c is expected for superconductors with low T_c's. Thus, we chose an optimally doped LSCO sample, $La_{1.85}Sr_{0.15}CuO_4$. We carried out precise lattice parameter measurements between 15 K and room temperature using a conventional x-ray powder diffractometer. We detected a change in strain perpendicular to the CuO_2 plane in the superconducting phase, which could be explained by the coupling between the strain and the superconducting gap. The strain of MgB_2 was also analysed by considering the coupling. To the best of our knowledge, this is the first indication of the coupling between the superconducting order parameter and the strain.

2. Experimental details

$La_{1.85}Sr_{0.15}CuO_4$ samples were prepared by a ceramic solid-state reaction. Appropriate amounts of La_2O_3, $SrCO_3$ and CuO were mixed and calcined in air at 950 °C for 20 h, then pulverized, pressed into pellets and sintered in air at 1000 °C for 40 h. The obtained products were then ground, pressed into pellets again, and sintered in air at 1050 °C for 40 h. The samples were cooled to room temperature in a furnace.

The electric resistance of a sample was measured by a conventional four-probe method with a current of 1 mA. Au wire probes were attached to bar-shaped ceramic samples using Ag paste. The resistance slightly increased at around 70 K and disappeared at about 35 K.

X-ray diffraction patterns were obtained using a Rigaku X-ray diffractometer, RINT2500, with a graphite counter monochromator and an X-ray generator with a rotating Cu anode. The generator was operated at 50 kV and 300 mA. A powder sample was obtained by grinding the ceramics. A platelike powder sample was mounted on a sample holder made of copper. The sample was fixed in a closed-cycle He gas refrigerator mounted on the diffractometer. The sample was cooled from room temperature to 15 K. The diffraction patterns between 20° and 140° were measured at a scanning speed of $2\theta = 0.4°/\text{min}$. Data were collected at every $2\theta = 0.02°$. The diffraction patterns were analysed by the Rietveld method to obtain accurate lattice parameters using the computer program RIETAN-2000 [6]; calculations were carried out by a conjugate direction method. $La_{1.85}Sr_{0.15}CuO_4$ shows tetragonal–orthorhombic structural phase transition at about 180 K [7]. We used the space groups $I4/mmm$ (No. 139) [8] and Cmca (No. 64) [9] for the tetragonal and orthorhombic phases, respectively.

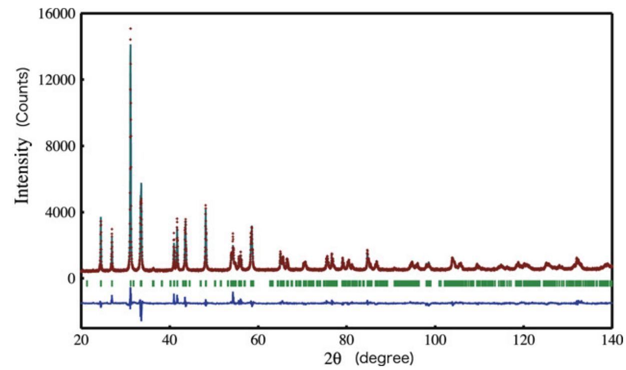

Fig. 1. Observed x-ray powder diffraction pattern and best-fit Rietveld refinement profile for orthorhombic $La_{1.85}Sr_{0.15}CuO_4$ at 15 K.

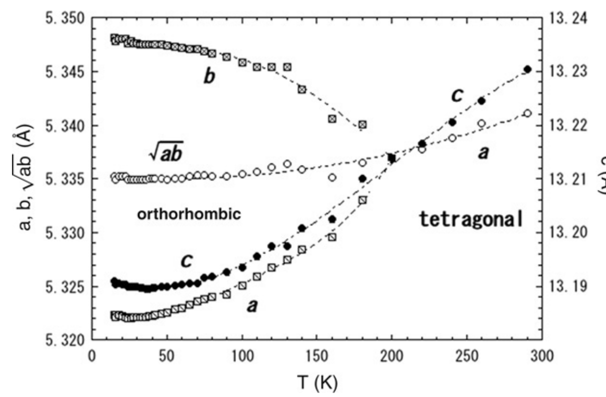

Fig. 2. Lattice parameters a, b, $(ab)^{1/2}$ and c of $La_{1.85}Sr_{0.15}CuO_4$ vs temperature based on X-ray powder diffraction measurements. The orthorhombic phase lattice parameter c is determined along the direction of c in the tetragonal phase to enable an easy comparison. The parameter a in the tetragonal phase is increased by a factor of $\sqrt{2}$ for easy comparison with a, b and $(ab)^{1/2}$ of the orthorhombic phase. Standard deviations are smaller than the symbols. Lines serve as visual guides.

3. Results and discussion

The result of the profile fit at 15 K for $x = 0.15$ is shown in Fig. 1, as an example. There are no clear impurity peaks. The obtained lattice parameters are delineated in Fig. 2 as a function of temperature. Tetragonal–orthorhombic structural phase transition, which produces a superstructure, occurs at around 180 K. The orthorhombic lattice parameter c is determined along the direction of the tetragonal lattice parameter c in Fig. 2 to enable an easy comparison of the lattice parameters. The tetragonal lattice parameter a shown in Fig. 2 is increased by a factor of $\sqrt{2}$ for easy comparison with a, b and $(ab)^{1/2}$ of the orthorhombic phase. Standard deviations are smaller than the symbols in Fig. 2. A distinct change in the lattice parameter c can be observed near the superconducting transition temperature.

The lattice parameters c of the tetragonal and orthorhombic phases are shown in Fig. 3 as a function of temperature along with the electric resistance for comparison. The lattice parameter is expected to show saturation at low temperatures if superconducting phase transition does not occur as the