Pressure-induced isostructural phase transition in $Bi_2Sr_2CaCu_2O_{8+\delta}$ *

ZHANG Jian-Bo(张建波)[1] TANG Ling-Yun(唐玲云)[1] ZHANG Jiang(张弓)[1] QIN Zhen-Xing(秦振兴)[1]
ZENG Xiao-Jing(曾小金)[1] LIU Jing(刘景)[2] WEN Jin-Sheng[3] XU Zhi-Jun[3]
GU Genda[3] CHEN Xiao-Jia(陈晓嘉)[1]

[1] Department of Physics, South China University of Technology, Guangzhou 510640, China
[2] Institute of High Energy Physics, Chinese Academy of Science, Beijing 100049, China
[3] Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, Upton, New York 11973, USA

Abstract: The high-pressure structures of an underdoped cuprate superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ have been studied by synchrotron X-ray diffraction at pressures up to 36.5 GPa. We find that this superconductor retains its orthogonal structure with the space group Amaa in the pressure range studied. Upon compression, both the a and b axes first shrink monotonically up to 17.4 GPa from their ambient pressure values and keep these behaviors with positive compressibilities up to 36.5 GPa after experiencing expansion with negative compressibilities in the pressure regime between 17.4 and 23.7 GPa. However, the c axis decreases continuously with increasing pressure with a slow change at about 23.7 GPa. The results indicate an isostructural phase transition starting at 17.4 GPa and a structural collapse at around 23.7 GPa.

Key words: cuprate superconductors, structural properties, high pressure, synchrotron X-ray diffraction

PACS: 61.05.cp, 74.72.Gh, 61.50.Ks **DOI:** 10.1088/1674-1137/37/8/088003

1 Introduction

Recently, there has been a great interest and effort in the search for superconductors with a higher transition temperature and better performance. High-pressure experiments play a significant role in this field and provide important information for understanding the mechanism of superconductivity [1]. For instance, the high-pressure technique led directly to the discovery of $YBa_2Cu_3O_{7-\delta}$ (Y-123) [2] with the superconducting transition temperature T_c above the liquid nitrogen boiling temperature, one of the most important high-T_c superconductors (HTSCs). And a record high T_c was obtained in $HgBa_2Ca_2Cu_3O_{8+\delta}$ at pressure of 32 GPa [3]. Remarkably, pressure-induced superconductivity has also been found in the newly discovered iron-based compounds [4–6].

Previous high pressure experiments on Bi-based HTSCs have shown rich physical properties related to the Cu-O layer structures. In the early work, both Klotz and Schilling [7] and Chen et al. [8] have shown a non-monotonic pressure behavior in $Bi_2Sr_2CaCu_2O_{8+\delta}$ over the whole doping regime, indicating that the pressure dependence of T_c is a result of the competition between the carrier density and pairing interaction strength. This idea was first proposed theoretically by Chen et al. [9] and confirmed from the recent muon spin rotation experiments [10]. The latter investigation on the optimally doped trilayer $Bi_2Sr_2CaCu_3O_{10+\delta}$ demonstrated a dramatic enhancement of the superconductivity by pressure-driven competition in electronic order [11]. Such competition takes place at different CuO_2 planes of the compound. On the other hand, the pressure-induced superconductivity has also been found in non-superconducting $Bi_{1.98}Sr_{2.06}Y_{0.68}CaCu_2O_{8+\delta}$ sample [12]. The effects of pressure on the superconductivity depend on many ingredients, such as oxygen order, crystallization and electronic structures [1], many of those remain unclear. Among them the structural property is essential for understanding the physical properties. Unfortunately, the pressure-dependent structural property has not been confirmed for these Bi-based HTSCs. A thorough investigation of the structural properties of a pure Bi-Sr-Ca-Cu-O system without intergrowth at high pressures has been absent since the discovery of these HTSCs.

In this paper we present the results of high-pressure studies on an underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$($T_c$=45 K) single crystals measured by a synchrotron powder X-ray diffraction at room temperature. It is found that the c-axis shrinks monotonically with increasing pressure.

Received 24 October 2012, Revised 19 November 2012

∗ Supported by Cultivation Fund of the Key Scientific and Technical Innovation Project, Ministry of Education of China (708070), and U. S. DOE BES (DE-AC02-98CH10886)

Strikingly, upon compression, both the a and b axes first shrink below 17.4 GPa, and then expand at pressures ranging from 17.4 GPa to 23.7 GPa, after which these axes continue to shrink. These results indicate an isostructural phase transition starting at 17.4 GPa and a complete transformation to a collapsed orthorhombic phase above 23.7 GPa.

2 The experiment details

Samples of single crystal $Bi_2Sr_2CaCu_2O_{8+\delta}$ were grown by a floating zone technique in a strong thermal gradient to stabilize the direction of solidification using a stoichiometric ratio (Bi:Sr:Ca:Cu=2:2:1:2) of actions as described elsewhere [13] and ground to fine powder for the experiments. X-ray diffraction patterns were obtained at the Beijing Synchrotron Radiation Facility (BSRF). A monochromatic X-ray beam with a wavelength of 0.6199 Å was used. High pressure was created by a symmetric diamond anvil cell (DAC) with a pair of 300 μm culet anvils. A hardened stainless steel gasket was indented, and a hole of 120 μm in diameter was drilled in the center as the sample chamber. Methanol/ethanol (volume ratio 4:1) liquid was loaded into chamber as the pressure medium. The pressure was determined by the shift of the fluorescence line from a tiny ruby chip situated next to the sample. X-ray diffraction patterns were collected by a Mar345 image plate at pressures up to ~36.5 GPa and at room temperature. The 2-D patterns were integrated into one dimensional XRD patterns with Fit2D software [14]. To investigate the crystal structure of each phase, the diffraction patterns obtained at selected pressures were fitted using the Le Bail method with GSAS software [15].

3 Results and discussion

The angle-dispersive powder X-ray diffraction data for an underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ with T_c of 45 K at various pressures are shown in Fig. 1. With the increase of pressure, the diffraction peaks at about 13° (up arrow) first move to a high angle from ambient pressure up to 17.4 GPa, and then move to a low angle up to 23.7 GPa, after that it does not change significantly. The diffraction peaks between 12° (down arrow) and 13° show obvious changes that merge at about 23.7 GPa. These results indicate a phase modification around 23.7 GPa. Le Bail fits of the data show that diffraction patterns could be clearly indexed using the orthogonal structure with the space group Amaa [16] up to 36.5 GPa for $Bi_2Sr_2CaCu_2O_{8+\delta}$.

Figure 2 demonstrates a typical Le Bail fitting of the synchrotron powder X-ray data of an underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ at pressure of 4.6 GPa. Obviously, the agreement between the observed X-ray diffraction pattern and fitting spectrum is quite good. We also attempt to fit the highest pressure phase with the orthogonal structure and the results between the observed and the calculated profiles provide satisfactory fits. These

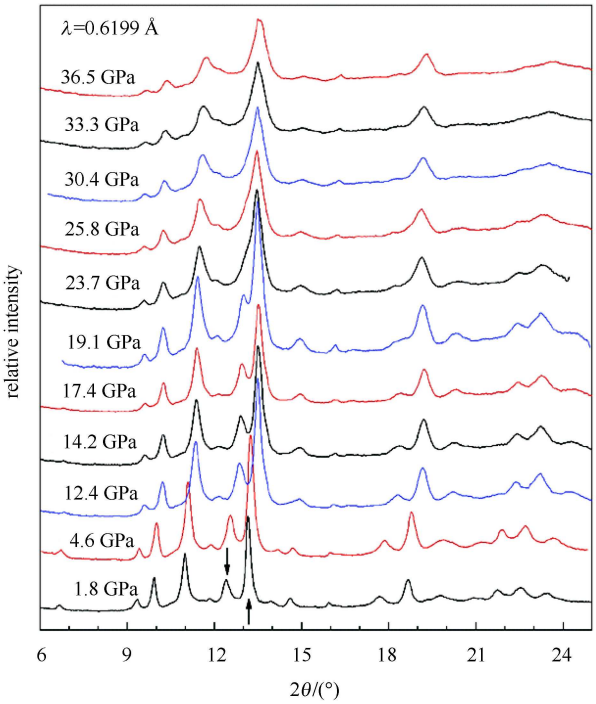

Fig. 1. The integrated synchrotron X-ray diffraction patterns of an underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ at various pressures up to 36.5 GPa. The arrows indicate the peak positions.

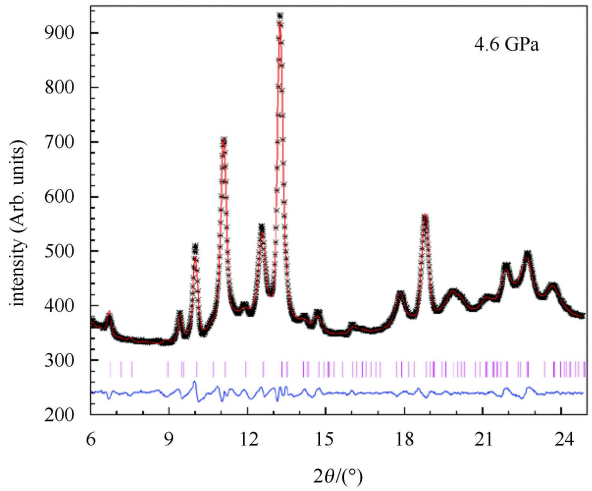

Fig. 2. The observed X-ray diffraction pattern (solid symbols), Le Bail fit (upper continuous line), and difference between the observed and calculated profiles (bottom blue line) obtained after Le Bail fitting of an underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ at 4.6 GPa with the space group of Amaa. The middle sticks refer to the peak positions.

results follow that $Bi_2Sr_2CaCu_2O_{8+\delta}$ remains in the orthorhombic structure at the pressure regime studied.

Figure 3 shows the pressure dependence of the lattice parameters along the a, b and c axes. The three lattice parameters decrease with increasing pressure below 17.4 GPa. With the further increase of pressure, both the a and b axes expand with a negative compressibility behavior up to 23.7 GPa, after which the compressibility becomes positive again. On the other hand, the c axis exhibits a rapid reduction with increasing pressure below 23.7 GPa; while this shrinkage slows down above 23.7 GPa. These results indicate an isostructural phase transition starting at 17.4 GPa. When the applied pressure is higher than 23.7 GPa, the structure completely transforms to a collapsed orthorhombic (CO) phase with the same space group Amaa.

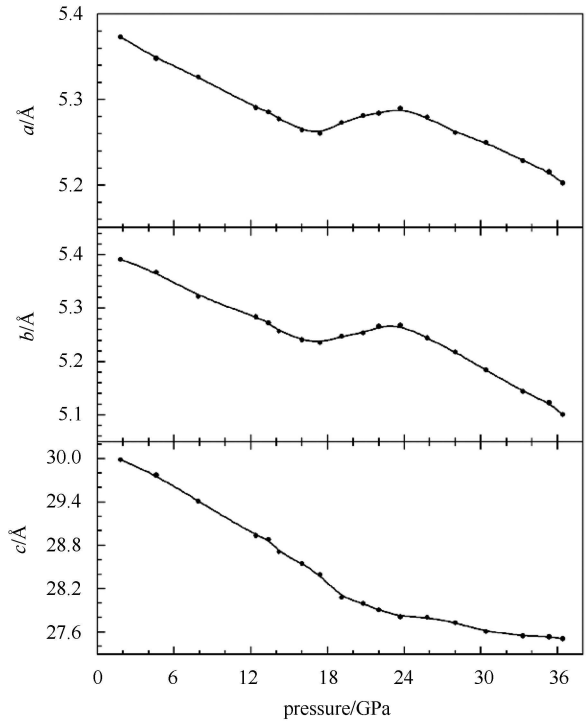

Fig. 3. The lattice parameters of the a, b and c axes of an underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ in the orthogonal phases as a function of pressure up to 36.5 GPa.

Figure 4 shows the measured pressure-volume (P-V) equation of state for an underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ at room temperature. As can be seen, the unit-cell volume decreases with pressure in both the low- and high-pressure regions and keeps a constant in between. The two volume compression regions are the the orthorhombic (O) and collapsed orthorhombic (CO) phases. The lines are the fitting results of the O and collapsed CO phases using the third-order Birch-Murnaghan equation of state [17]:

$$P = \frac{3}{2}B_0\left[(V/V_0)^{-7/3}-(V/V_0)^{-5/3}\right] \times\left\{1+\frac{3}{4}(B'-4)\left[(V/V_0)^{-2/3}-1\right]\right\},$$

where B_0 is the bulk modulus at zero pressure, B' is the first pressure derivative of the bulk modulus at zero pressure, and V_0 is the volume at ambient pressure. A least-square fit to the measured P-V data yields B_0=114.9±6.4 GPa for the O phase with a fixed B'=4.0, while V_0=221.1±1.05 Å^3. We also obtain B_0=126.96±11.3 GPa and V_0=222.98±2.54 Å^3 for the CO phase.

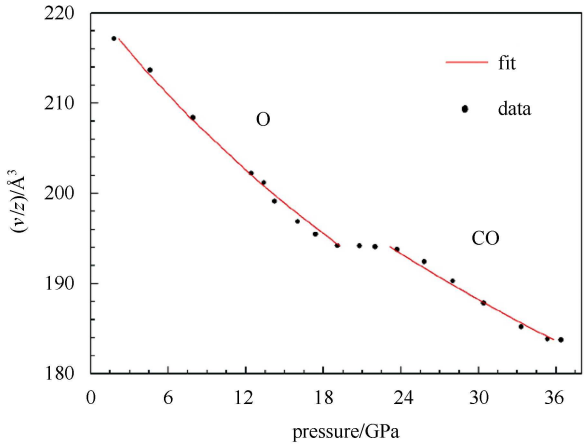

Fig. 4. Pressure dependence of the unit-cell volume of an underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ up to 36.5 GPa. The solid points are the measured data and the curves are the P-V equation of state fits to the two sets of data, i.e., the O phase (low-pressure region) and the CO phase (high-pressure region).

It has been well accepted that the superconductivity in cuprates can be produced either through chemical substitutions or by pressure. Therefore, the crystal and electronic structures of these superconductors are always modified substantially through these effects [18–20]. Any lattice distortions induced by the application of either internal chemical or external hydrostatic pressure always lead to the change of the transition temperature T_C [21–23]. Thus this structural feature is important for understanding the role of lattice effects on high-T_C superconductivity [24]. The obtained isostructural phase transitions are very similar to those reported in the iron-based superconductors [25–28]. For iron-based superconductors, the parent compound $BaFe_2As_2$ was reported to undergo a phase transition from a tetragonal to a collapsed tetragonal phase at 27.0 GPa [25].

For another sister system $CaFe_2As_2$, a similar transition occurs at 2.0 GPa [25]. The analogical occurrence of structural phase transition from a normal tetragonal phase to a collapsed tetragonal phase has been widely reported in $EuFe_2As_2$ [26], $Nd(O_{0.88}F_{0.12})FeAs$ [27], and $BaFe_{1.8}Ni_{0.2}As_2$ [28]. The investigation of the relationship between the structural transitions and electronic transports demonstrates that the superconductivity disappears while the phase transition happens [25–27]. It is thus argued that such anomalous compressibility effects may be a clue to the mechanism of superconductivity in unconventional layered superconductors [29]. However, such anomalous pressure behaviors have seldom been reported on other kinds of superconductors such as cuprates. The observation of the phase transition in the studied $Bi_2Sr_2CaCu_2O_{8+\delta}$ indicates that it is not an exclusively property in ion-based superconductors. Thus the investigation of pressure effects may provide a way for a better understanding of the hidden mechanism of superconductivity in HTSCs.

4 Conclusions

We have investigated the structural properties of an underdoped compound $Bi_2Sr_2CaCu_2O_{8+\delta}$ at high pressures up to 36.5 GPa through the powder synchrotron X-ray diffraction technique. With increasing pressure, both the a and b axes exhibit an anomalous behavior while the c axis drastically decreases. Our results suggest an isostructural phase transition from the O phase to the CO phase at around 23.7 GPa. These structural behaviors may lead to unexpected superconducting properties in these cuprate superconductors.

We acknowledge the Beijing Synchrotron Radiation Facility (BSRF) for the provision of beam time.

References

1 Robert Schrieffer J. Handbook of High-Temperature Superconductivity: Theory and Experiment. Springer Science+Business Media, LLC, 2007. 427–461
2 WU M K, Ashburgn J R, Torng C J, Hor P H, Meng R L, GAO L, HUANG Z J, WANG Y Q, CHU C W. Phys. Rev. Lett., 1987, **58**: 908
3 GAO L,XUE Y Y, CHEN F, XIONG Q, MENG R L, Ramirez D, CHU C W, Eggert J H, MAO H K. Phys. Rev. B, 1994, **50**: 4260
4 Torikachvili M S, Bud ko S L, NI N, Canfield P C. Phys. Rev. Lett., 2008, **101**: 057006
5 Alireza P L, Chris Ko Y T, Gillett J, Petrone C M, Cole J M, Lonzarich G G, Sebastian S E. J. Phys. Condens. Matter, 2009, **21**: 012208
6 Okada H, Igawa K, Takahashi H, Kamihara Y, Hirano M, Hosono H, Matsubayashi K, Uwatoko Y. J. Phys. Soc. Jpn, 2008, **77**: 113712
7 Klotz S, Schilling J S. Physica C, 1993, **209**: 499
8 CHEN X J, Struzhkin V V, Hemley R J, MAO H K, Kendziora C. Phys. Rev. B, 2004, **70**: 214502
9 CHEN X J, LIN H Q, GONG C D. Phys. Rev. Lett., 2000, **85**: 2180–2183
10 Maisuradze A, Shengelaya A, Amato A, Pomjakushina E, Keller H. Phys. Rev. B, 2011, **84**: 184523
11 CHEN X J, Struzhkin V V, YU Y, Goncharov A F, LIN C T, MAO H K, Hemley R J. Nature, 2010, **466**: 950-953
12 Cuk T, Zocco D A, Eisaki H, Struzhkin V, Grosche F M, Maple M B, SHEN Z X. Phys. Rev. B, 2010, **81**: 184509
13 GU G D, Takamuku K, Koshizuka N, Tanaka S. Journal of Crystal Growth, 1993, **130**: 325–329
14 Hammersley A P. Fit 2d, ESRF, Grenoble, France. 1998
15 Larson A C, Von-Dreele R B. GSAS-General Structure Analysis System. Report LAUR 86-748. Los Alamos National Laboratory, USA. 1994
16 GAO Y, Coppens P, Cox D E, Moodenbaugh A R. Acta Cryst. A, 1993, **49**: 141-148
17 Birch F. Phys. Rev., 1947, **71**: 809
18 Dagotto E. Science, 2005, **309**: 257
19 Orenstein J, Millis A J. Science, 2000, **288**: 468
20 Lampakis D, Liarokapis E, Panagopoulos C. Phys. Rev. B, 2006, **73**: 174518
21 Gantis A, Calamiotou M, Palles D, Lampakis D, Liarokapis E. Phys. Rev. B, 2003, **68**: 064502
22 Calamiotou M, Gantis A, Margiolaki I, Palles D, Siranidi E, Liarokapis E. J. Phys. Condens. Matter, 2008, **20**: 395224
23 Calamiotou M, Gantis A, Lampakis D, Siranidi E, Liarokapis E, Margiolaki I, Conder K. EPL, 2009, **85**: 26004
24 Calamiotou M, Gantis A, Siranidi E, Lampakis D, Karpinski J, Liarokapis E. Phys. Rev. B, 2009, **80**: 214517
25 Mittal R, Mishra S K, Chaplot S L, Ovsyannikov S V, Greenberg E, Trots D M, Dubronvinsky L, Su Y, Brueckel T, Matsuishi S, Hosono H, Garbarino G. Phys. Rev. B, 2011, **83**: 054503
26 Uhoya W, Tsoi G, Vohra Y K, McGuire M A, Sefat A S, Sales B C, Mandrus D, Weir S T. J. Phys. Condens. Matter, 2010, **22**: 292202
27 ZHAO J G, WANG L H, DONG D W,LIU Z G, LIU H Z, CHEN G F, WU D, LUO J L, WANG N L, YU Y, JIN C Q, GUO Q Z. J. Am. Chem. Soc., 2008, **130**: 13828
28 JIA F J, YANG W G, LI L J, XU Z A, CHEN X J. Physica C, 2012, **474**: 1–4
29 Sefat A S. Rep. Prog. Phys., 2011, **74**: 124502