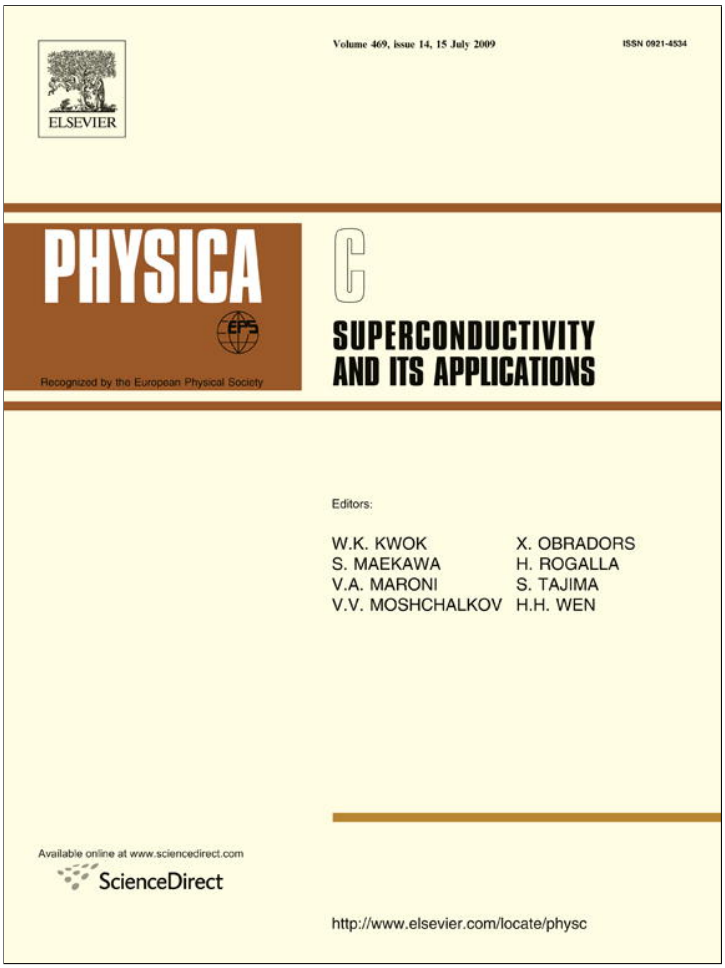

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Pressure tuned crystal structure in $NdBa_2Cu_3O_{6+\delta}$ superconductor

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ABSTRACT

The high-pressure angle-dispersive X-ray diffraction experiments on the $NdBa_2Cu_3O_{6+\delta}$ superconductor were performed from ambient to above 30 GPa at room temperature. The structure analysis based on the Rietveld refinement methods shows the different pressure dependence for the bond length between the basal-plane copper of the pyramids to the apical oxygen (denoted Cu(2)–O(1)) and bond length between basal-plane copper to plane oxygen (denoted Cu(2)–O(2,3)). The ambient bulk modulus B_0 is derived as 127 GPa. A possible correlation between Cu(2)–O(1) and T_c was discussed.

1. Introduction

The application of high-pressure has opened up new vistas in developing novel high temperature superconductor (HTS) materials or improving their physical properties [1–9]. It is well known that the superconducting transition temperature T_c of layered copper oxides can be tuned by the application of high-pressure. For example, the T_c of Hg1223 increases from 134 K at ambient pressure to 164 K at above 30 GPa [3]. However, the higher T_c values obtained must be accompanied with the structural evolution. For instance, in the $YBa_2Cu_3O_{6+\delta}$ (Y-123) system, studies on the correlation between T_c and the structural changes has revealed that the strong increase in T_c with δ is accompanied by a marked reduction in the distance from the basal-plane copper of the pyramids to the apical oxygen (denoted Cu(2)–O(1)) [10]. This was interpreted as signaling a charge-transfer from the basal-planes to the O–Cu–O chains, such that the hole-carrier density in the basal-planes increases. Further detailed studies of the structure as a function of oxygen content (δ) show a very intimate correspondence between the variations of T_c and Cu(2)–O(1) with δ [11]. The correlation between T_c and the structural evolution under high-pressure was performed in the Y-124 system [12]. The results showed some unusually large structural changes, most notably in the Cu(2)–O(1) bond length, suggesting that in this case the evolution in T_c could be attributed to the significant charge-transfer effects. Subsequently, pressure dependence of T_c in the $NdBa_2Cu_3O_{6+\delta}$, which is isomorphous to $YBa_2Cu_3O_{6+\delta}$ as shown in Fig. 1, indicated that T_c monotonically increases with pressure to 6 GPa [13]. It is suggested that pressure indirectly affects the carrier concentration in addition to its direct effects on the interlayer distance. In this paper, we report the results of X-ray diffraction with synchrotron radiation on bulk $NdBa_2Cu_3O_{6+\delta}$ sample with pressure up to above 30 GPa. We got the detailed information on lattice parameters and the equation of state at room temperature up to 18 GPa by refining the structure using Rietveld method. It shows an unusual pressure tuned evolution of the crystal structure.

2. Experimental

The $NdBa_2Cu_3O_{6+\delta}$ sample was prepared by traditional solid state reaction of high purity (99.9%) reagents of Nd_2O_3, CuO and $BaCO_3$ with the Nd, Ba, and Cu atoms in the ratios 1:2:3. The mixtures of starting materials were pressed into pellets and sintered at 950 °C for 24 h. The sintered pellets were then reground and sintered at 950 °C in flowing oxygen for 36 h and slowly cooled down to room temperature. The process was repeated until single phase

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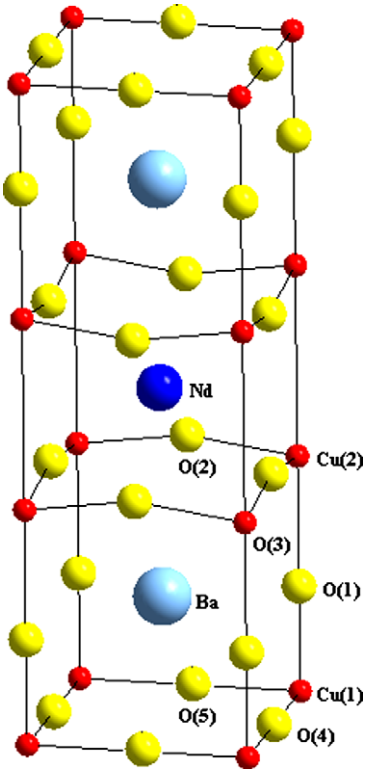

Fig. 1. Schematic view of the crystal structure of $NdBa_2Cu_3O_{6+\delta}$.

was obtained. The as-grown sample was examined by using X-ray diffraction patterns with Cu K_α radiation. The patterns showed the sample to be pure single phase having the same orthorhombic structure as $YBa_2Cu_3O_{6+\delta}$. The superconducting transition temperature T_c, measured by the Meissner effect, is 87 K for $NdBa_2Cu_3O_{6+\delta}$ sample.

The in site high-pressure X-ray angle-dispersive diffraction experiment on $NdBa_2Cu_3O_{6+\delta}$ sample was carried out at room temperature using a diamond anvil cell (DAC) at Beijing Synchrotron Radiation Facility (BSRF). The culet of diamond is 500 μm in diameter and the hole in a T301 stainless steel gasket is 250 μm in diameter. The gasket was preindented from 300 μm thickness to 30 μm thickness before drilling a sample hole. The powder sample is loaded into the hole in the gasket with silicon oil as pressure-transmitting medium that can provide a relative good hydrostatic pressure environment. A small ruby chip was put aside the sample for pressure calibration [14]. The wavelength of incident X-ray is 0.6199 Å. The diffraction patterns were collected with an image plate. The images were integrated with the *fit2d* program [15]. The structural parameters and interatomic distances were obtained by Rietveld refinement of the diffraction pattern in the range of $3° < 2\theta < 25°$ using GSAS program package [16].

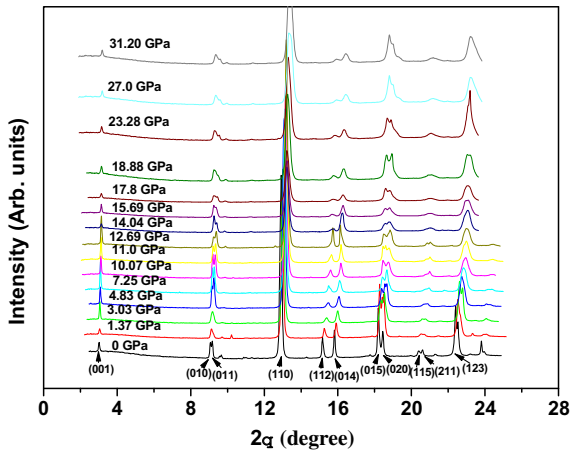

Fig. 2. Angle-dispersive X-ray diffraction spectra for $NdBa_2Cu_3O_{6+\delta}$ sample at room temperature.

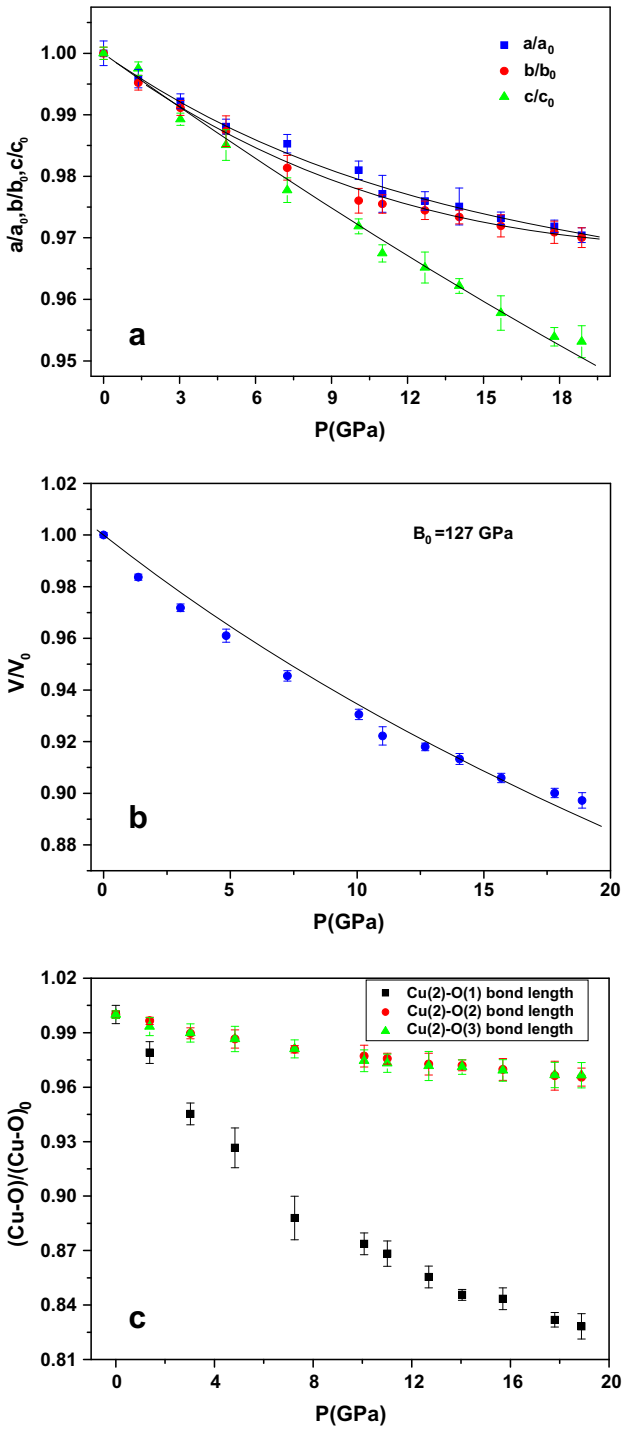

Fig. 3. The relationship of lattice parameters (a), volume compressibility (b) and Cu(2)–O(1), Cu(2)–O(2) and Cu(2)–O(3) bond length compressibility (c) verse pressure for $NdBa_2Cu_3O_{6+\delta}$ sample.

3. Results and discussion

The diffraction peaks agreed well with powder diffraction patterns of the orthorhombic unit cell. All diffraction peaks shift to higher-angle direction with increasing pressure as shown in Fig. 2. It is evidenced in our experiment that the orthorhombic phase is stable at least up to 30 GPa. When pressure returns to ambient, the peaks almost recover to their original sites. The detailed structure parameters were obtained up to 18 GPa (above this the pattern quality becomes low) by the Rietveld refinement using GSAS program package. The relationships of lattice parameters and volume compressibility versus pressure for $NdBa_2Cu_3O_{6+\delta}$ sample are shown in Fig. 3a and b. It can be clearly seen in Fig. 3a that the crystal lattices are anisotropically compressed, i.e., the structure is more easily compressed along *c* axis than in *ab* plane. Fitting the data to the Birch–Murnaghan equation of state:

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

where the pressure derivative $B_0' = 4$, the bulk modulus B_0 = 127 GPa is obtained.

Fig. 3c shows the changes in Cu(2)–O(1), Cu(2)–O(2) and Cu(2)–O(3) bond lengths with pressure. It is found that these bond lengths decrease nearly linearly with increasing pressure up to 18 GPa. The Cu(2)–O(2) bond compressibility is close to that of Cu(2)–O(3) bond, whereas, a much larger compressibility in Cu(2)–O(1) bond length was observed, suggesting highly anisotropic compression in this sample. It is noted in the copper oxide superconductors that the change in the bond length between the in-plane Cu and apical oxygen, i.e., the Cu(2)–O(1) bond length, is believed to be responsible for the charge-transfer from the CuO chain to the CuO_2 plane. The experimental study on Y-124 system suggested that the charge carrier concentration increases with increasing pressure within the pressure range 0–18 GPa [17,18], suggesting the existence of a correlation between the charge carrier concentration and the change in the Cu(2)–O(1) bond length. Also, pressure dependence of T_c in the $NdBa_2Cu_3O_{6+\delta}$ showed that T_c monotonically increases with pressure up to 6 GPa [13]. More recently, we measured the pressure dependence of critical temperature T_c for $NdBa_2Cu_3O_{6+\delta}$ sample up to a pressure of 13 GPa using a cryogenic diamond anvil cell in our lab. The results show that the onset critical temperature increases from 87 K at ambient pressure at least to 8 GPa. The large increase of T_c at low pressure can be explained by means of a large change of the number of charge carriers in the CuO_2 planes as a function of pressure that leads to an optimal doping of the $NdBa_2Cu_3O_{6+\delta}$ superconductor. Further increase pressure will overdope the $NdBa_2Cu_3O_{6+\delta}$ superconductor that in turn decreases T_c. Therefore it is expected that there will be an optimal doping pressure where T_c goes up to the maximum. Further increasing pressure will cause the decrease of T_c. Thus, pressure can be a useful tool in understanding the importance of interplanar coupling for high-T_c superconductivity. However, at present stage, there is no any evidence for the direct dependence of T_c on the carrier density change caused by compressing Cu(2)–O(1) bond length. It will be an open but very interesting topic to develop a technique that can be applied to detect the in situ pressure induced carrier density change.

4. Conclusion

Using the synchrotron radiation technique, we have studied the detailed information on lattice structure and the equation of state at room temperature up to above 30 GPa on bulk $NdBa_2Cu_3O_{6+\delta}$ sample. It indicates an anisotropic compression along *c* axis versus *ab* plane of in $NdBa_2Cu_3O_{6+\delta}$ sample. We suggest that pressure-induced apical oxygen bond length changes can tune T_c by modifying carrier through charge-transfer between charge reservoir and CuO_2 plane.

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