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Structure refinements of superconducting and nonsuperconducting $La_{1.82}Ca_{1.18}Cu_2O_{6\pm\delta}$ from neutron-diffraction data

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The crystal structures of superconducting and nonsuperconducting $La_{1.82}Ca_{1.18}Cu_2O_{6\pm\delta}$ synthesized under O_2 pressures of 400 and 2 atm were refined by Rietveld analysis of neutron-powder-diffraction data. These samples contained no impurities and their observed and calculated diffraction patterns were in excellent agreement. In both samples, Ca and La preferentially occupied, respectively, a 2a site in eightfold coordination and a 4e site in ninefold coordination; a slightly higher ordering was observed in the superconducting compound. An apical oxygen site was almost fully occupied. A trace of excess oxygen between two CuO_2 planes was detected in the superconducting compound. Cu-O(1) and Cu-O(2) bond lengths differed a little between the two samples. Increases in cation ordering and in interstitial oxygen might be important factors determining superconductivity in this system.

INTRODUCTION

Bulk superconductivity has recently been achieved in "2:1:2:6-type" copper oxides synthesized under high O_2 pressure—in compounds not doped with Sr ($La_{2-x}Ca_{1+x}Cu_2O_{6-x/2+\delta}$ with $0.08 \le x \le 0.25$) (Refs. 1-3) and in Sr-doped compounds [$La_{2-x}Sr_xCaCu_2O_6$ and $La_{2-x}(Ca_{1-y}Sr_y)_{1+x}Cu_2O_{6-x/2+\delta}$].[4-7] The relations between crystal structure and superconductivity in superconducting $La_{1.6}Sr_{0.4}CaCu_2O_{5.94}$ (Ref. 8) and $La_{1.8}Sr_{0.2}CaCu_2O_6$ (Ref. 9) and in weakly superconducting $La_2CaCu_2O_{6.04}$ (Ref. 10) have been investigated by use of neutron powder diffraction. Because the 2:1:2:6 compounds are not superconducting if they are conventionally synthesized in air or in 1-atm O_2, special attention has been given to oxygen stoichiometry but no consistent results have been obtained. This may be due to the difficulty of synthesizing superconductors free from impurity phases, and the Sr-containing superconductors prepared by Cava *et al.*[8] and Sakurai *et al.*[9] evidently contained small amounts of impurities. Furthermore, no detailed comparison of crystal structures between superconducting and nonsuperconducting 2:1:2:6 compounds has yet been reported.

The present paper reports neutron-diffraction studies of impurity-free $La_{1.82}Ca_{1.18}Cu_2O_{6\pm\delta}$. The structures of both superconducting and nonsuperconducting compounds have been refined precisely, and structural differences between them have been compared in detail.

EXPERIMENTS AND STRUCTURAL REFINEMENTS

Samples were synthesized from La_2O_3, $CaCO_3$, and CuO powders with purities higher than 99.9%. Nonsuperconducting $La_{1.82}Ca_{1.18}Cu_2O_{6-\delta}$ was prepared by firing the mixture at 1060 °C for 50 h under 2 atm of flowing O_2. Superconducting $La_{1.82}Ca_{1.18}Cu_2O_{6+\delta}$ was obtained by sintering the nonsuperconducting compound again at 1080 °C for 100 h in 20% O_2+80% Ar at a total pressure of 2000 atm using a furnace for hot isostatic pressing (HIP).

Neutron-diffraction data were collected at room temperature on a time-of-flight (TOF) neutron powder diffractometer, HRP, at the KENS pulsed-spallation neutron source at the National Laboratory for High Energy Physics.[11] The gate width was appropriately set at 4–16 μs, depending on the TOF.

Structure parameters were refined by using RIETAN (Ref. 12) for the Rietveld analysis of TOF neutron-diffraction data on the basis of $I4/mmm$ space group.[13,14] The crystal structure of the 2:1:2:6 compound is shown in Fig. 1. Wycoff positions are 2a (0,0,0) for La(1) and Ca(1), 4e (0,0,z) for La(2), Ca(2), Cu, and O(2), 8g (0,$\frac{1}{2}$,z) for O(1), and 2b (0,0,$\frac{1}{2}$) for O(3). Anisotropic thermal parameters U_{ii} were assigned to all the sites except the interstitial 2b site of O(3) whose isotropic thermal parameter B was arbitrarily fixed at 1 Å^2 because of its very low occupancy. Refinement of the occupancy for the O(3) site in the nonsuperconducting com-

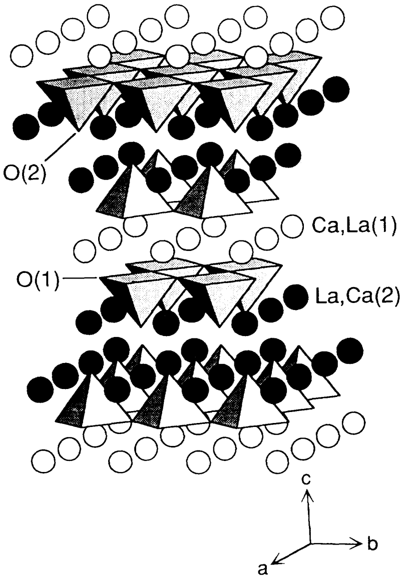

FIG. 1. Crystal structure of $La_{2-x}Ca_{1+x}Cu_2O_6$. The $[CuO_5]$ pyramidal planes are the electrically active components.

pound gave a very small negative value, so it was fixed at zero in the final refinement. The site occupancies g's were refined under the following linear constraints: $g(Ca(1)) = 1 - g(La(1))$, $2g(La(2)) = 1.82 - g(La(1))$, and $2g(Ca(2)) = 1.18 - g(Ca(1))$. The coherent scattering lengths used for the Rietveld analysis were 8.24 (La), 4.90 (Ca), 7.718 (Cu), and 5.803 fm (O).[15]

RESULTS AND DISCUSSION

Figure 2 shows the temperature dependence of electrical resistivity for the superconducting and nonsuperconducting compounds. Both compounds had almost the same electrical resistivity at temperatures above 100 K but their electrical resistivities differed significantly at lower temperatures. The superconducting compound had a T_c (onset) of about 60 K and a T_c (zero) of about 49 K. The bulk nature of this compound's superconductivity was confirmed by magnetic susceptibility measurements (Fig. 3). The flux exclusion due to diamagnetization shielding was almost 100%, and the Meissner volume fraction was more than 15% of that expected for an ideal diamagnet.

The final refinable structure parameters of the superconducting and nonsuperconducting compounds are listed in Table I, and the observed, calculated, and difference patterns for superconducting $La_{1.82}Ca_{1.18}Cu_2O_{6+\delta}$ are shown in Fig. 4. No signs of impurities were detected in the neutron-diffraction patterns of the two samples, and very small-R factors show excellent agreement between observed and calculated intensities

Lattice parameters, selected interatomic distances and O-Cu-O bond angles are listed in Table II. For easier comparison, fractional changes r are also shown which are defined as $100\,(l_s - l_n)/l_n$, where l is the lattice parameter or interatomic distance, and subscripts s and n, respectively, denote superconductor and nonsuperconductor.

Cation ordering at the 2a and 4e sites is important for determining the location of doped holes. When La is at 4e sites and Ca is at 2a sites, the Madelung potential of the apical O(2) atom relative to that in the CuO_2 plane is positive and holes are thus doped on the plane.[16] When the La and Ca atoms are disordered, this Madelung potential is negative and the doped holes enter the apical O(2) site. Superconductivity appears when the doped holes enter the CuO_2 plane.[16,17] The difference in coherent scattering lengths between La (8.24 fm) and Ca (4.90 fm) is large enough to obtain reliable information about the distribution of La^{3+} and Ca^{2+} ions between the 2a and 4e sites. The superconducting compound has

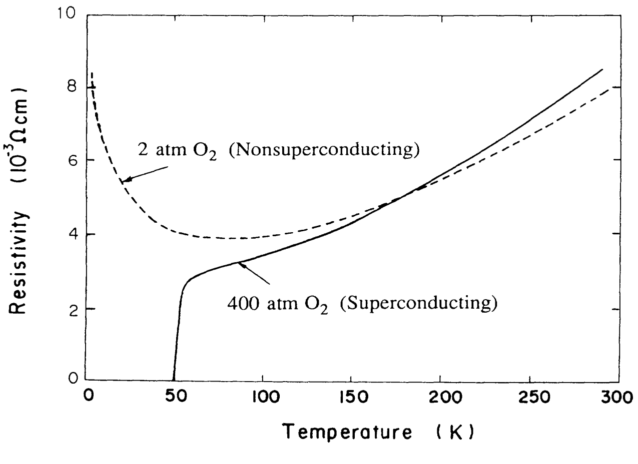

FIG. 2. Electrical resistivity vs temperature for superconducting and nonsuperconducting $La_{1.82}Ca_{1.18}Cu_2O_{6\pm\delta}$.

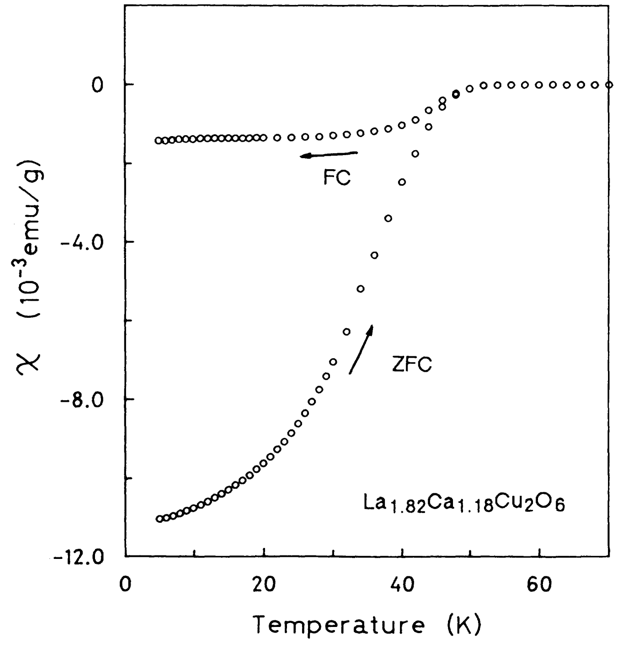

FIG. 3. Magnetic susceptibility vs temperature for superconducting $La_{1.82}Ca_{1.18}Cu_2O_{6+\delta}$. Susceptibility was measured in zero-field-cooling (ZFC) and field-cooling (FC) conditions.

TABLE I. (Top) Crystal data for superconducting $La_{1.82}Ca_{1.18}Cu_2O_{6.014\pm0.007}$. The symbol g is the site occupancy, U_{ii}'s are anisotropic thermal parameters when the temperature factor is defined as $\exp[-2\pi^2(h^2a^{*2}U_{11}+k^2b^{*2}U_{22}+l^2c^{*2}U_{33})]$, and B_{eq} is the equivalent isotropic thermal parameter. Estimated standard deviations shown in parentheses refer to the least significant digit(s). R factors are as follows: $R_{wp}=4.57\%$, $R_e=4.08\%$, $R_p=3.40\%$, $R_I=2.30\%$, and $R_F=1.81\%$. (Bottom) Crystal data for nonsuperconducting $La_{1.82}Ca_{1.18}Cu_2O_{5.99\pm0.02}$. R factors are as follows: $R_{wp}=4.99\%$, $R_e=3.83\%$, $R_p=3.62\%$, $R_I=2.84\%$, and $R_F=1.74\%$.

Atom	Site	x	y	z	g	U_{11} (Å^2)	U_{22} (Å^2)	U_{33} (Å^2)	B_{eq} (Å^2)
La(1)	2a	0	0	0	0.043	0.004 4(9)	$=U_{11}$	0.009 1(19)	0.47
Ca(1)	2a	0	0	0	0.957(15)	0.004 4(9)	$=U_{11}$	0.009 1(19)	0.47
La(2)	4e	0	0	0.175 99(7)	0.889	0.008 1(5)	$=U_{11}$	0.003 8(7)	0.53
Ca(2)	4e	0	0	0.175 99(7)	0.111	0.008 1(5)	$=U_{11}$	0.003 8(7)	0.53
Cu	4e	0	0	0.415 09(9)	1	0.003 0(3)	$=U_{11}$	0.008 1(9)	0.38
O(1)	8g	0	$\frac{1}{2}$	0.081 86(7)	1	0.003 2(5)	0.006 4(5)	0.013 5(8)	0.61
O(2)	4e	0	0	0.296 04(13)	1	0.025 9(7)	$=U_{11}$	0.005 6(9)	1.51
O(3)	2b	0	0	$\frac{1}{2}$	0.014(7)				
La(1)	2a	0	0	0	0.062	0.007 3(15)	$=U_{11}$	0.006(3)	0.53
Ca(1)	2a	0	0	0	0.94(2)	0.007 3(15)	$=U_{11}$	0.006(3)	0.53
La(2)	4e	0	0	0.175 86(11)	0.88	0.006 9(7)	$=U_{11}$	0.006 0(11)	0.52
Ca(2)	4e	0	0	0.175 86(11)	0.12	0.006 9(7)	$=U_{11}$	0.006 0(11)	0.52
Cu	4e	0	0	0.415 04(13)	1	0.003 3(5)	$=U_{11}$	0.009 0(13)	0.41
O(1)	8g	0	$\frac{1}{2}$	0.082 15(11)	1	0.003 8(8)	0.007 2(8)	0.015 8(12)	0.71
O(2)	4e	0	0	0.295 8(2)	0.995(12)	0.027 9(13)	$=U_{11}$	0.006 3(15)	1.63
O(3)	2b	0	0	$\frac{1}{2}$	0				

slightly larger occupancies of La(2) at the 4e site and Ca(1) at the 2a site than the nonsuperconducting one. Similar results were obtained from the Rietveld analysis of x-ray powder diffraction data.[3,6] However, the difference in g(Ca(1)) between the two samples is so little that their g(Ca(1)) values agree with each other within estimated standard deviations. The effective ionic radii for La^{3+} and Ca^{2+} ions in eight coordination are 1.16 Å and 1.12 Å, respectively,[18] which suggests that the Ca,La(1)-O(1) bond length decreases with increasing g(Ca(1)). In fact, the r values in Table II indicate that the Ca,La(1)-O(1) bond length decreases to the largest extent by the HIP treatment. This finding gives indirect evidence in favor of the higher ordering of La^{3+} and Ca^{2+} ions in the superconductor.

The O(1) site was fully occupied in both superconducting and nonsuperconducting compounds. The apical O(2) site of the superconducting $La_{1.82}Ca_{1.18}Cu_2O_{6+\delta}$ was also fully occupied, which is not true for $La_{1.6}Sr_{0.4}CaCu_2O_{5.94}$ (Ref. 8) and $La_{1.8}Sr_{0.2}CaCu_2O_6$ (Ref. 9). The occupancy of O(2) for the nonsuperconductor was refined to be slightly less than 1 in the present

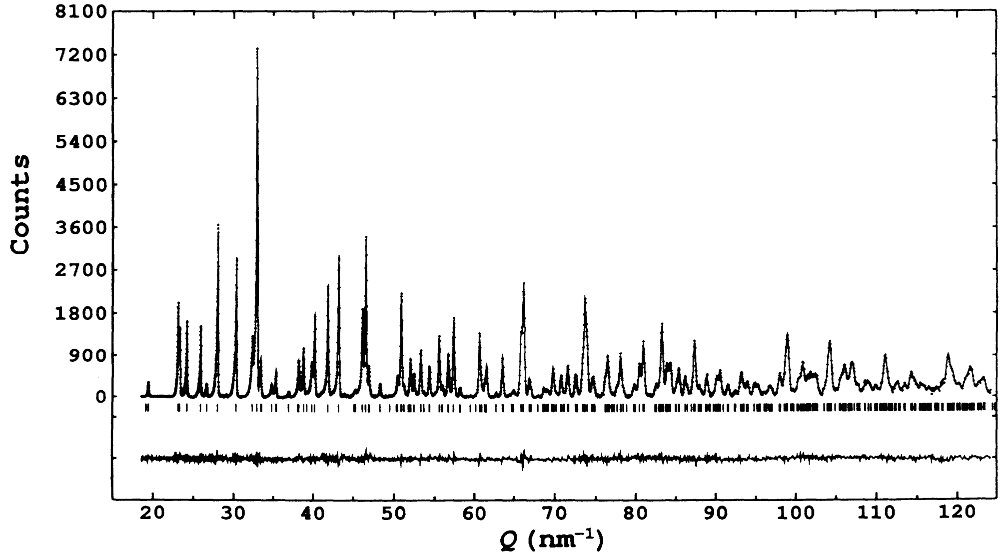

FIG. 4. Rietveld refinement patterns for superconducting $La_{1.82}Ca_{1.18}Cu_2O_{6+\delta}$ plotted against Q $(=2\pi/d)$. The background is subtracted. Plus marks show observed neutron-diffraction intensities, and the solid line represents calculated intensities. The curve at the bottom shows the difference between the observed and calculated intensities in the same scale.

TABLE II. Lattice parameters *a* and *c* (Å), selected interatomic distances (Å), and O-Cu-O bond angles (°) in superconducting and nonsuperconducting $La_{1.82}Ca_{1.12}Cu_2O_{6\pm\delta}$. Fractional changes, *r*, in them are also listed. Estimated standard deviations in parentheses refer to the least signficant digit(s). Footnotes a–d are symmetry codes. $r=100(l_s-l_n)/l_n$, where *l* is the lattice parameter or interatomic distance, and subscripts *s* and *n* denote superconductor and nonsuperconductor, respectively.

	Superconducting	Nonsuperconducting	*r* (%)
a	3.816 04(6)	3.821 99(7)	−0.16
c	19.421 4(3)	19.416 4(4)	0.03
Ca,La(1)-O(1) (×8)	2.483 6(9)	2.489 2(14)	−0.22
La,Ca(2)-O(1) (×4)	2.642 4(14)	2.639 (2)	0.13
La,Ca(2)-O(2^a) (×4)	2.752 5(5)	2.757 9(7)	−0.20
La,Ca(2)-O(2) (×1)	2.332 (3)	2.329 (4)	0.13
Cu-O(1^a) (×4)	1.908 9(1)	1.911 8(1)	−0.15
Cu-O(2) (×1)	2.312 (3)	2.315 (5)	−0.13
Cu-Cu^b (×4)	3.298 (3)	3.299 (5)	−0.03
O(1^a)-Cu-O(1^c)	89.945 (4)	89.953 (6)	−0.01
O(1^a)-Cu-O(1^d)	176.44(14)	176.7(2)	−0.15
O(1^a)-Cu-O(2)	91.78(7)	91.64(11)	−0.15

[a] $\frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}-z$

[b] $x, y, 1-z$

[c] $\frac{1}{2}-y, \frac{1}{2}+x, \frac{1}{2}-z$

[d] $-\frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}-z.$

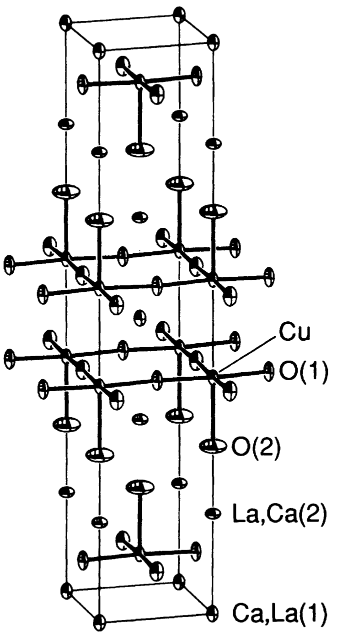

FIG. 5. ORTEP-II drawing of superconducting $La_{1.82}Ca_{1.18}Cu_2O_{6+\delta}$. The thermal ellipsoids are drawn as 95% probability surfaces. Cu and O atoms are connected with bonds.

analysis: 0.995(12). Within the estimated standard deviation, however, the O(2) site in the nonsuperconductor can also be regarded as fully occupied. Nearly full occupation of the O(2) site must lead to the more excellent superconducting properties of $La_{1.82}Ca_{1.18}Cu_2O_{6+\delta}$, compared with those of $La_{1.6}Sr_{0.4}CaCu_2O_{5.94}$ (Ref. 8) and $La_{1.8}Sr_{0.2}CaCu_2O_6$ (Ref. 9). As Fig. 5 shows, anisotropic thermal vibrations of the O(2) atom in both superconductor and nonsuperconductor are very marked along the *a* and *b* axes. This implies that the O(2) atom at this site not only vibrates significantly in directions parallel to the CuO_2 plane but also deviates statically from the ideal 4e position. However, such anisotropic thermal vibration or atomic displacement is often observed in rocksalt-type planes in superconducting copper oxides and should not impair superconductivity.

A slight amount of oxygen [g=0.014(7)] is intercalated at the O(3) site between two CuO_2 planes of the superconductor but not of the nonsuperconductor. Slight amounts of excess oxygen between two CuO_2 planes are also observed in superconducting $La_{1.8}Sr_{0.2}CaCu_2O_6$ (Ref. 9) and weakly superconducting $La_2CaCu_2O_{6.04}$ (Ref. 10). Therefore, the presence of interstitial oxygen may be essential for the superconductivity of the 2:1:2:6-type compounds.

Antiferromagnetic Néel temperatures for Ar-annealed $La_{1.82}Ca_{1.18}Cu_2O_{6-\delta}$ and hydrogenated $La_{1.9}Ca_{1.1}Cu_2O_6H_x$ are higher than 300 K and those for $La_{1.82}Ca_{1.18}Cu_2O_{6\pm\delta}$ synthesized in 0.2–2 atm O_2 are around 20 K;[19,20] antiferromagnetic order disappears in superconductors.[20,21] In layered compounds, the Néel temperature is generally evaluated by the relation $kT_N \sim J_\perp^{\text{eff}}\xi_{2D}^2$, where $J_\perp^{\text{eff}}$ is the effective coupling between planes, and ξ_{2D} is the magnetic correlation length within a layer.[22,23] The small amount of interstitial oxygen atoms may frustrate interplane coupling $J_\perp^{\text{eff}}$ and destroy three-dimensional (3D) long-range antiferromagnetic order by bridging the CuO_2 planes, or they may frustrate two-dimensional antiferromagnetic Cu^{2+}-Cu^{2+} spin correlations within CuO_2 planes by increasing hole carriers in them. In fact, Hall-coefficient measurements[24] showed that hole concentrations of the superconductor and nonsuperconductor were 1.4×10^{21} and 1×10^{21} cm^{-3} at 100 K, respectively. Superconductivity in this system may appear as a result of such frustrations for antiferromagnetic order.

However, a large amount of excess oxygen destroys superconductivity of the 2:1:2:6-type compounds[25] by disturbing the regularity and two-dimensionality of the CuO_2 planar network. In reality, $La_{1.85}Sr_{1.15}Cu_2O_{6.24}$, which has a considerable amount of excess oxygen between two CuO_2 planes, is not superconducting even if synthesized under a high-O_2 pressure.[3]

In the superconductor, *a* was slightly smaller and *c* was slightly larger than their values in the nonsuperconductor. The equatorial Cu-O(1) bond of the superconductor was slightly shorter than that of the nonsuperconductor, which directly reflects the smaller lattice parameter *a* in the superconductor because the Cu-O(1) bond is nearly parallel to *a*. The Cu-O(2) bond lengths had the same tendency, which is, however, rather ambiguous because of their large statistical uncertainties. The shrinkage of the Cu-O(1) and Cu-O(2) bonds must reflect the increased hole concentration in the CuO_2 plane and contribute to the occurrence of superconductivity. In fact, the bond valence sum for Cu was 2.330 for the superconductor and 2.311 for the nonsuperconductor. The difference between them is not large because of the small changes in the Cu-O bond lengths.

The oxygen contents $6\pm\delta$ calculated from the occupancies of the O(1), O(2), and O(3) sites were 6.014 ± 0.007 for the superconducting compound and 5.99 ± 0.02 for the nonsuperconducting compound. The difference in oxygen content corresponds to an increase in Cu valence as much as 0.024 in the superconductor. This increment is fairly close to the difference in bond valence sum between the two samples: 0.019. These results clearly show that the hole concentration on the CuO_2 plane is increased by the HIP treatment.

CONCLUSIONS

The structures of superconducting and nonsuperconducting $La_{1.82}Ca_{1.18}Cu_2O_{6\pm\delta}$ free from impurities have been refined precisely, and structural differences between them have been compared in detail. In the superconducting compound, the site occupancies of La(2) at the 4e site and Ca(1) at the 2a site were estimated to be slightly higher than in the nonsuperconductor, and interstitial O(3) atoms between the two CuO_2 planes were detected. These are thought to be important factors determining superconductivity because the hole concentration in the CuO_2 plane is increased by these changes. In particular, a trace of interstitial oxygen atoms is believed to play an important role because such oxygen atoms destroy antiferromagnetic order either directly by bridging CuO_2 planes three-dimensionally or indirectly by increasing the hole concentration in the CuO_2 plane. The apical O(2) site is nearly 100% occupied, which leads to superconducting properties superior to those of the 2:1:2:6-type oxides containing Sr. The valences of Cu evaluated on the basis of the bond valence sums and oxygen contents indicate that the HIP treatment does increase the hole concentration on the CuO_2 plane. The comparison of crystal structures between superconducting and nonsuperconducting compounds at low temperatures could be valuable because electrical properties differ greatly at low temperatures and only slightly at temperatures higher than 100 K.

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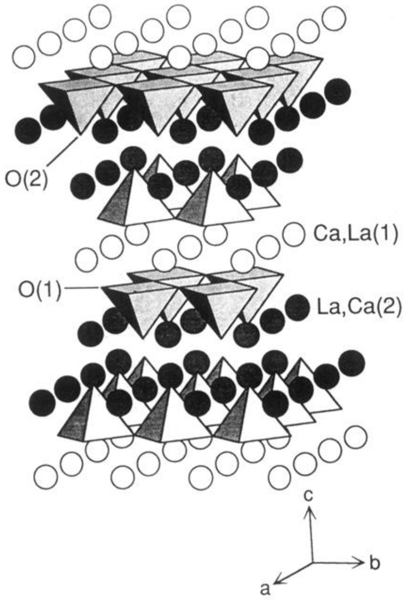

FIG. 1. Crystal structure of $La_{2-x}Ca_{1+x}Cu_2O_6$. The $[CuO_5]$ pyramidal planes are the electrically active components.