Effect of The Number of Holes P_{sh} and Heat Treatments on the Critical Temperature T_c in High T_c Superconductors

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Abstract— We report here on the preparation, X-ray diffraction with Rietveld refinement and the effect of heat treatments in $Y_{1-x}Sm_xBaSrCu_3O_{6+z}$. Each sample was subject to two types of heat treatment: oxygen annealing [O] and argon annealing followed by oxygen annealing [AO]. When x increase from 0 to 1, the ratio a/b increases and $T_c[O]$ decreases. However, $T_c[AO]$ decreases until x=0.2 and after it increases with a/b by 5.3 K to 84.6 K for x=1 [AO]. Note that the crystalline parameter b is constant but a (and c) increases indicating an increase of the number of oxygen atoms by chain (NOC) along a leading to a decreases of a/b(T_c)[O] toward a tetragonal structure. For each x, the [A0] heat treatment decreases a/b (for 0≤ x ≤1), T_c (for x>0.4). Note that for x=0.4, the surface of the sample s[O]=s[AO] with $T_c[O] \approx T_c[AO]$=81.4 K. Remarkable correlations were observed. A combination of several factors such as the decrease in $d[Cu_{(2)}-Cu_{(1)}]$; the increase in cationic and oxygen chain order; the effect of the number of holes p_{sh} in the $Cu(2)O_2$ plans and in-phase purity for the [AO] samples may account the observed data.

Keywords— High-T_c superconductors, Heat treatments, holes p_{sh}, T_c, surface ab, distance d[Cu(1)-Cu(2)], X- ray diffraction.

I. INTRODUCTION

The substitution of different atoms in the high critical temperature superconductor $YBa_2Cu_3O_{6+z}$ is an important method for obtaining essential information about superconductivity. The effects of these substitutions affect the number of the holes p in the $Cu(2)O_2$ superconducting plane. It has been proved experimentally that the optimum $Cu(2)O_2$ plane conditions in these cuprites are the result of the effect of these holes to attain a high critical temperature [1-4].

Several authors show that the critical temperature depends only on the ionic size of rare earth in the samples $LnBaSrCu_3O_{6+z}$ (Ln rare earth) [5-7]. We have studied the structural and superconducting properties of the superconductor $SmSrBaCu_3O_{6+z}$ [8]. This compound when annealed in oxygen at 450°C showed a tetragonal structure and a T_c of 79 K. When the same sample was heated in argon followed by oxygen annealing; we observed an orthorhombic structure and an increase of Tc by 6 K. So T_c depends also on heat treatment.

In order to study the role played by the yttrium and barium planes, and to find out the factors and conditions which govern the superconductivity in these compounds; we have investigated the structural and superconducting properties of $(Y_{1-x}Sm_x)(SrBa)Cu_3O_{6+z}$. Indeed, we found that the influence of argon heat treatment on these properties depended on the concentration of Sm(x) and T_c depends on the number of holes p_{sh} in the $Cu(2)O_2$ plans.

II. EXPERIMENTAL TECHNIQUES.

The polycrystalline samples have been prepared by solid-state sintering of the respective oxides and carbonates. The chemicals were of 99.999% purity except in the case of $BaCO_3$ which was 99.99% pure. Sm_2O_3, $SrCO_3$, $BaCO_3$ and CuO were thoroughly mixed in required proportions and calcined at 950°C in air for a period of 12-18h. The resulting product was ground, pelletized and heated in air at 980°C for a period 16-24h. This was repeated twice. The pellets were annealing in oxygen at 450°C for a period of 60-72h and furnace cooled. This was denoted as sample [O] for each x. XRD data of the sample ware collected with Philips diffractometer fitted with a secondary beam graphite monochromator and using CuK_α (40 kV/20 mA) radiation. The angle 2θ was varied from 20° to 120° in steps of 0.025° and the courting time per step was 10 sec. The XRD specters were refined with Rietveld refinement [9].

Superconducting transitions were checked by measuring both the real χ' and the imaginary χ'' parts of the AC susceptibility as a function of temperature in a field of 0.11 Oe and at a frequency of 1500 Hz.

For each x, the same sample [O] was then heated in argon at 850°C for about 12h, cooled to 20°C and oxygen was allowed to flow instead of argon and the sample was annealed at 450°C for about 72h. This sample is denoted as [AO]. XRD and AC susceptibility measurements were performed on a part of this sample.

III. RESULTS AND DISCUSSION

As example, the measured XRD patterns and calculated with Rietveld refinement in the case of $SmSrBaCu_3O_{6+z}$ ([O] and [AO]) are shown in figure 1. In general the samples were well crystallized and the reflections were sharper after the [AO] heat treatment. The orthorhombic splitting was also influenced by the [AO] treatment. Some weak unidentified impurity peaks α (at 2θ=31°) were seen

in the [O] samples. They disappeared after the [AO] heat treatment. This indicates an improvement of crystallographic quality of the samples [AO].
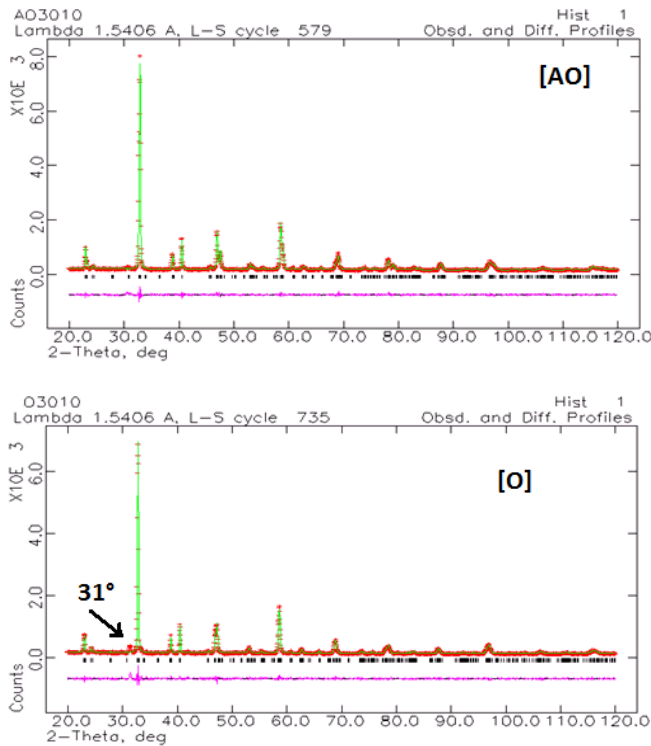

Fig. 1 : XRD pattern of SmSrBaCu$_3$O$_{6+z}$, observed, calculated with Rietveld refinement and difference profiles for sample [O] and sample [AO].

In order to determine the coordinates of these atoms (i.e. the positions of the atoms in the unit cell), we chosen the reference (a,b,c) with origin at Y/Sm site. The atoms of the basal plan have the following fixed coordinated: Cu(1) (0.5,0.5,0.5), O(4) (0,0.5,0.5) and O(5)(0.5,0,0.5), while those of the other atoms O(1), O(2), O(3), Cu(2) and Sr/Ba vary along the z axis. The positions of the atoms in Y$_{1-x}$Sm$_x$SrBaCu$_3$O$_{6+z}$ are schematized in figure 2.

Figure 3 illustrates the evolution of the lattice parameters a, b, c, the surface s as function of the x(Sm) and the heat treatment. Figure3. (a) shows that the two curves c[O] and c[AO] are identical. It indicates that the parameter c does not depend on the heat treatment but depends only on the composition x(Sm). The parameter c increases with x in agreement with the fact that r(Sm^{3+})=0.965 Å is superior to that r(Y^{3+})= 0.893 Å.

The effect of the heat treatment on the surface s(x) =ab of the unit cell is remarkable. The figure 3(b) shows that s[AO]>s[O] for x≤0,5 with T$_c$[AO]<T$_c$[O]. This effect is reversed for x > 0.5. We notice that for x=0.4 s[AO] =s[O] with T$_c$[AO] =81.5K almost equal to T$_c$ [O] =81.3K. These results show that T$_C$ depends on the surface s, i.e. of order/disorder of oxygen in the basal plane. We also have obtained the same curve of T$_c$ as function of s and the volum as a function of x and the heat treatment in figure 5. This shows again that the heat treatment does not influence the parameter c.

Figure 4(a) shows the a/b ratio as function of x (Sm) and the heat treatment. The increase of a/b[O] from 0.983 (a≠b) for x = 0 to 0.997≈1 (with a=b) for x = 1 indicates a structural phase transition from orthorhombic to tetragonal. While for the samples [AO], a/b[AO] increases slowly from 0.9804 for
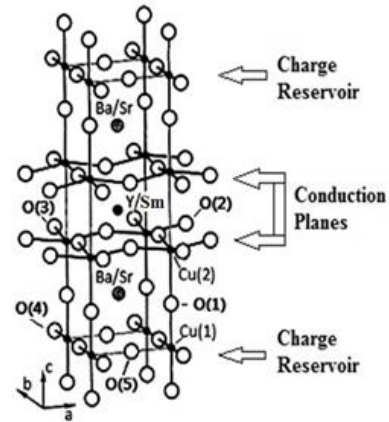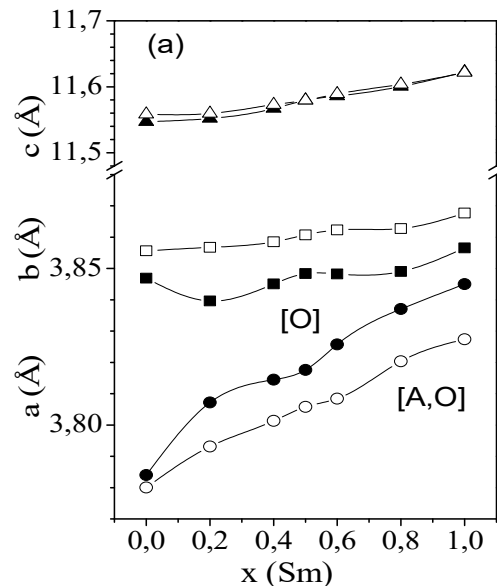

Fig. 2 : The unit cell of the compound Y$_{1-x}$Sm$_x$SrBaCu$_3$O$_{6+z}$.

x=0 (for YBaSrCu$_3$O$_{6+z}$) to 0.9896 for x=1 (SmBaSrCu$_3$O$_{6+z}$) with an orthorhombic symmetry. For each x, the heat treatment [AO] decreases the a/b ratio. Thus, the heat treatment influences the parameters a and b, but not c, i.e. the order/disorder of oxygen in the basal plan ab, and consequently impacts the number of the holes in the Cu(2)O$_2$ copper planes. When x increase from 0 to 1, the a/b[O] ratio increases and T$_c$[O] decreases as seen in Figure 4(b).

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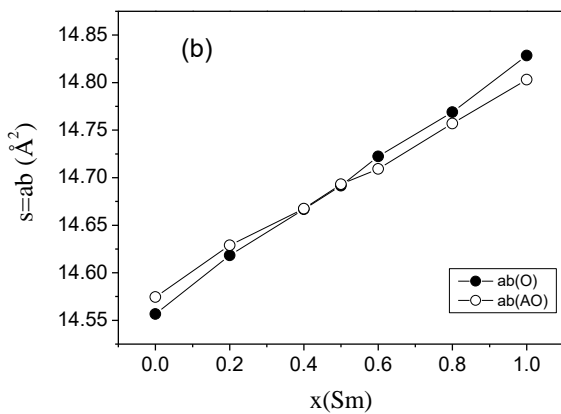
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Fig. 3 : Variation of the parameters a, b and c (a) and surface s (b) of $Y_{1-x}Sm_xSrBaCu_3O_{6+z}$ as function of x and the heat treatment.
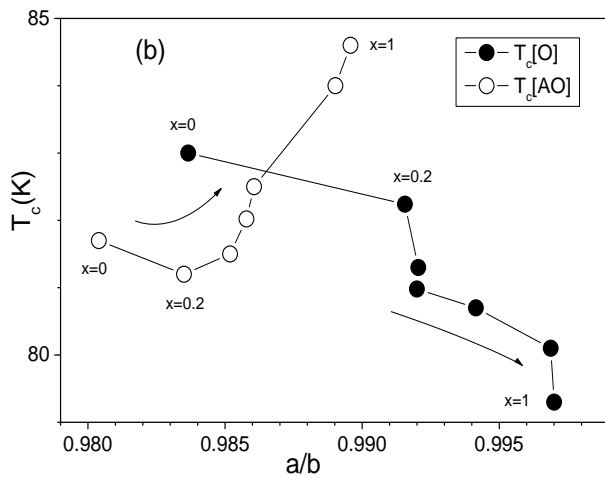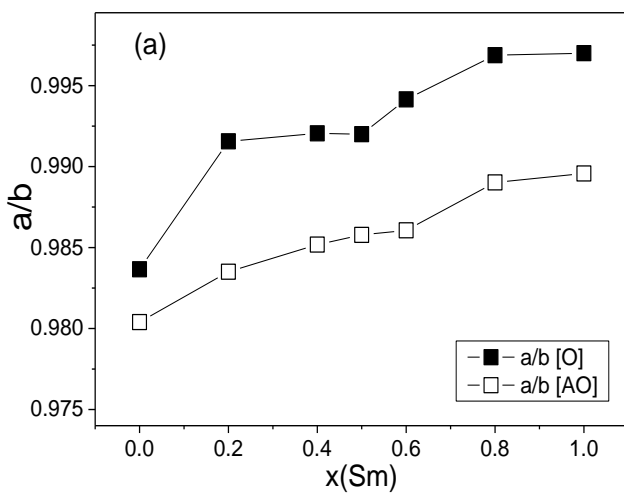

Fig. 4 : (a):The a/b ratio of $Y_{1-x}Sm_xSrBaCu_3O_{6+z}$ as function of x and the heat treatment. (b): Variation of the ratio a/b as a function of Tc and heat treatments of $Y_{1-x}Sm_xSrBaCu_3O_{6+z}$.

The high critical temperature T_c of superconductors' oxides strongly depends on the concentration of the holes on the two-dimensional layers $Cu(2)O_2$. The universal relation between standardized T_c ($\tau_c = T_c/T_{cmax}$) and the concentration p_{sh} of the holes in the $Cu(2)O_2$ plane of superconductors oxides (La214 , Y123, Bi2212, Bi2223, Tl2201 and Tl1212) shows that T_c independent of the considered sample [1].

The existence of the plateau for $0.12 < p_{sh} < 0.25$, in which the critical temperature is maximal ($\tau=1$) [1], is observed experimentally. Particularly in the universal correlation between T_c and n_s/m^* (the ratio of the density of the holes and the effective mass) given by Uemura et al [10]. An increase in T_c, of a system to another, is related to a decrease of m^* and an increase of n_S.

A correlation between the critical temperature and the oxygen arrangement in the layers of head tank for the compound $(Cu,C)Ba_2Ca_2Cu_3O_{9-\delta}$ was given by N. Iliev et al. [11]. It is based on the fact that the variation of the rate of oxygen in these layers influences the content of the holes (p_{sh}) in the plans of conduction $Cu(2)O_2$. Thus, M. R. Presland et al [12] obtained a parabolic relation. between T_c standardized $\tau_c = T_c/Tc_{max}$ and the concentration of the holes p_{sh}.

Typically, when doping rises from p=0.06 the critical temperature T_c increases from zero to attain its maximal value T_{cmax} at p=0.16. This is accompanied by the reduction of the pseudo gap energy E_g du to the depression in electron density of states. At critical doping level p=0.25, the pseudo gap phase eventually vanishes and further increase of doping is characterized by decrease of T_c and disappearance of superconductivity at p≈0.30.

The following empirical relationship between T_c and p has been found in experiments to hold for a wide class of high T_c cuprates. The determination of p_{sh}, is estimated by equation (1) from the T_c measured in a sample, where Tc_{max} is 93K in the case of cuprates [13].

$$T_c(p_{sh})=T_{cmax}[1-82.6(p_{sh}-0.16)^2] \qquad (1)$$

We have obtained a correlation between the number of the holes p_{sh} and the critical temperature T_c as function of x(Sm) and the heat treatment in $Y_{1-x}Sm_xBaSrCu_3O_{6+z}$ in (figure 6).

The distance d[Cu(2)-Cu(1)] between the copper Cu(2) of the $Cu(2)O_2$ plan and the copper Cu(1) of the chains as function of x and the heat treatment is shown in the figure 7. We obtained a remarkable correlation between the inverse of this distance (d^{-1}[Cu(1)-Cu(2)]) with T_c as a function of x and the heat treatment as seen in figure 8. In the unit cell (figure.2), the copper Cu(1) is fixed; therefore, the variation of this distance is the result of the displacement of copper Cu(2) along z.

For a given heat treatment, when the critical temperature $T_c(x)$ increases the distance d[Cu(1)-Cu(2)](x) decreases (d^{-1}[Cu(1)-Cu(2)] (x) increases) in Figure 7 and 8. The attraction force via the apical oxygen O(1) intermediate makes it possible to increase T_c. This apical oxygen plays the role the bridges linking charge reservoir and CuO_2 conducting layers for highs superconductors (HTS) [14].

The reduction of number of holes in the CuO_2 planes makes it possible to increase the parameter c in $Y_{1-x}Sm_xBaSrCu_3O_{6+z}$ [O] (Figure. 9). It is the same behavior of the figure obtained by Ruixing Liang et al [2] in the case the doping p of $YBa_2Cu_3O_{6+z}$ as a function of the lattice

parameter c. The c-direction unit cell length is the sum of bond lengths, $c = 2d[Cu(1)-O(1)]+d[Cu(2)-Cu(2)]+2d[Cu(2)-O(1)]$. The change in c is mainly caused

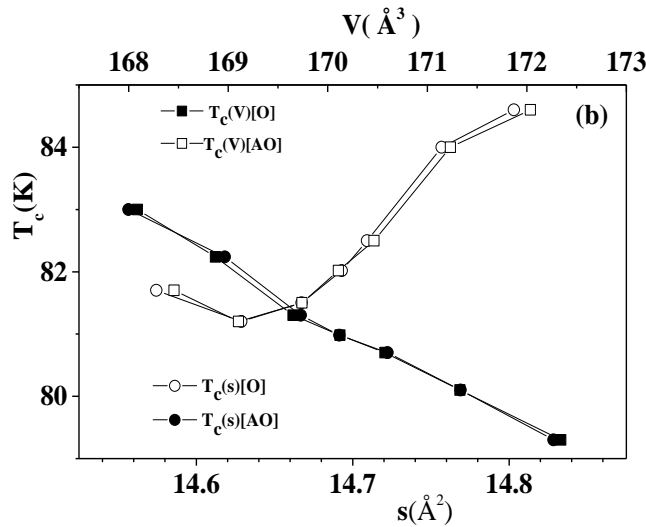

Fig. 5 : The critical temperature as function of the volume, the surface of the unit cell and the heat treatment in $(Y_{1-x}Sm_x)BaSrCu_3O_{6+z}$.
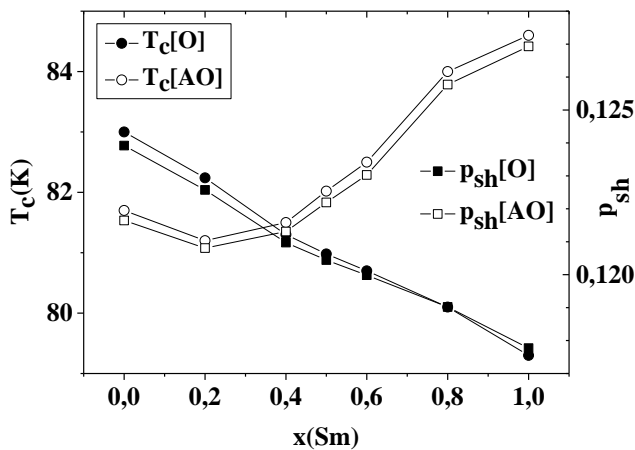

Fig. 6 : Correlation between the number of the holes p_{sh} the critical temperature as function of x(Sm) and the heat treatment in $Y_{1-x}Sm_xBaSrCu_3O_{6+z}$.

by the change in d[Cu(2)-O(1)] because it is much more sensitive to change in the oxygen content than other bond lengths [2]. This result can also be justified by the figures (6 and 8)[O], such that the parameter c[O] increases with the distance d[Cu(2)-Cu(1)][O]. Indeed the critical temperature $T_c[O]$ and $p_{sh}[O]$ increase when x decreases, but the distance d[Cu(2)-Cu(1)][O] decreases which also reduces the parameter c[O]. The parameter c increases when the oxygen content decreases in the basal plane of the samples $REBa_2Cu_3O_y$ (RE=Gd, Er) [15].

The latter decreases with the doping p [2]. The maximum critical temperature is obtained in the tetragonal structure with the constant crystal parameter a=0.385nm. In the compounds $REBa_2Cu_3O_7$ (RE=rare-earth elements) T_c=92K [3] and in the compound $SmBaSrCu_3O_{6+z}[O]$, T_c= 79.3K in the Cu(2)O$_2$ plane on the superconducting property by the influence on the parameter a ($a = 2d_{Cu(2)-O(2)} = 2d_{Cu(2)-O(3)}$), compared with that obtained by Wang et al. [5] (T_c = 80K).

This also shows that the role played by the number of holes.

The critical temperature T_c varies as a function of the n number of Cu(2)O$_2$ planes in $Ba_2Ca_{n-1}(CuO_2)n(O,F)_2$ [4]. It is maximal for n = 3 and constant from n = 5. It is evident that the crystal parameter c increases with the number n of the Cu(2)O$_2$ planes. This increase is linear in the case of $Sr_2Ca_{n-1}Cu_nOy$ (n = 3-7)[16]. Piyamas Chainok et al [17] synthesized the $YBa_mCu_{1+m}O_{(2m+3)-x}$ superconductors; m = 2, 3, 4, 5 that were Y123, Y134, Y145 and Y156 by solid state reaction. They found that the T_c^{onset} of Y123, Y134, Y145 and Y156 were at 97, 93, 91 and 85 K. The Y123 has two CuO$_2$ planes and one CuO chain. In 2009, Aliabadi et al [18] synthesized Y358 ($Y_3Ba_5Cu_8O_{18}$) superconductor by solid state reaction that becomes superconducting above 100 K with the lattice parameters a = 3.888 Å, b = 3.823 Å, c = 31.013 Å. The Y358 has crystal structure similar to Y123 with five CuO$_2$ planes and three CuO chains. So, the increase in the number n of Cu(2)O$_2$ planes and Cu(1)O chain have important effect on the T_c of YBaCuO superconductors.

Isovalent substitution doping (here substitution of Y^{+3} by Sm^{+3}) changes the number of holes in the Cu(2)O$_2$ plans, the chemical substitution unavoidably introduces disorder into the crystalline lattice due to random distribution of dopant
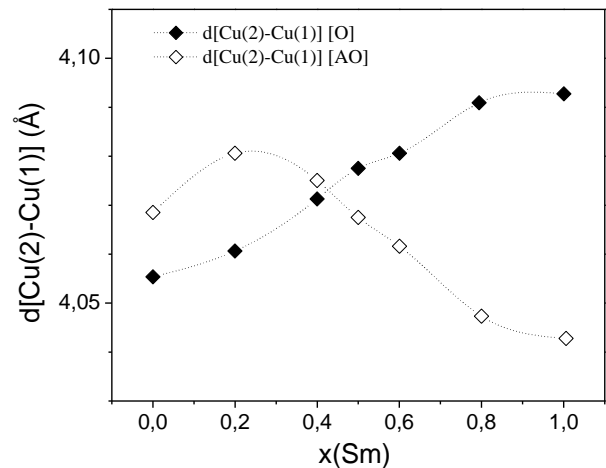

Fig. 7: The distance d[Cu(1)-Cu(2)] as function of x(Sm) and heat treatment in $Y_{1-x}Sm_xBaSrCu_3O_{6+z}$

atoms. The effect of the doping disorder on T_c has become a recent concern. This effect of holes p on T_c has been systematically studied for the cuprates based copper oxide superconductors by several authors [1 ,19].

This is identical to the model of transfer of the charge from the chains towards the Cu(2)O$_2$ plans. Thus, T_c increases while d[Cu(2)-Cu(1)] decreases. Indeed, the increase in the holes in the Cu(2)O$_2$ plan makes it possible to increase the force of repulsion between Cu^{2+} and (Y^{3+}/Sm^{3+}) cations which increase the distance d[Y/Sm–Cu(2)]. The Y/Sm atom is fixed in our unit cell while copper Cu(2) of plan moves towards copper Cu(1) of chain. Consequently, the distance d[Cu(1)-Cu(2)] decreases. The increase in holes in the Cu(2)O$_2$ plane decreases this distance and increases the critical temperature T_c (Figures 6 and 8). Finally, the effect of the concentration

of the mobile holes in the $Cu(2)O_2$ plane, on the structural and superconducting properties, is quite remarkable in our samples.

When x increases from 0 to 1, the cation and anion disorder increases (reduction of number Oxygen by Chain NOC [20]) in the samples [O]. Thus, the concentration p_{sh} of holes (or T_c) of these samples [O] decreases (figures 5 and 6). The treatment [AO] reduces the atomic disorders (increase in
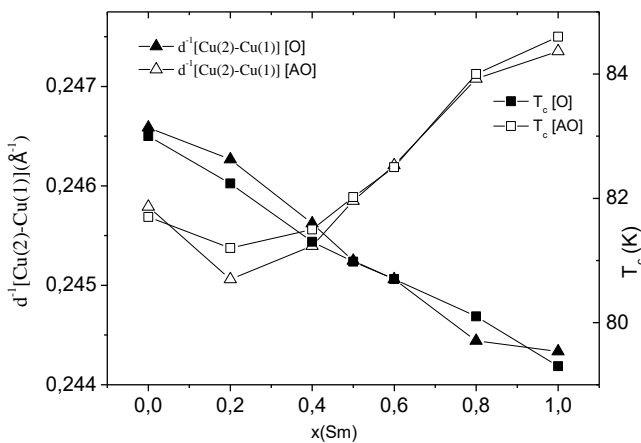

Fig. 8: The inverse of a distance $d^{-1}[Cu_{(1)}-Cu_{(2)}]$ and the critical temperature as function of x(Sm) and heat treatment in $Y_{1-x}Sm_xBaSrCu_3O_{6+z}$.
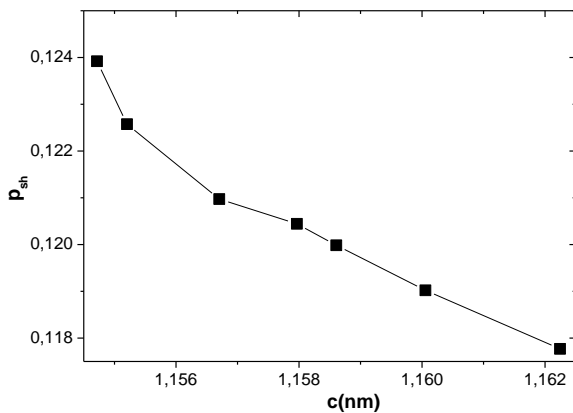

Fig. 9: p_{sh} of $Y_{1-x}Sm_xBaSrCu_3O_{6+z}$ [O] as a function of the lattice Parameter c.

the NOC), which increases p_{sh} (or T_c) [13, 20]. For a given x, the heat treatment [AO] increases p_{sh} and T_c for x ≥ 0.4. It should be noted here that, while x increases, the concentration p_{sh} of holes (or T_c) of samples [AO] decrease; in the first time, from x=0 to x=0.2 (like the case of sample [O]) and increases after.

Recently, V. Antal et al. [21] use argon-oxygen heat treatment to improve the superconducting properties in the $YBa_2(Cu_{1-x}Li_x)_3O_{7-\delta}$ samples.

We hold that parameter a increases with x and parameter b remains almost constant. The increase in parameter a is attenuates in the samples [AO]. The surface s increases linearly. When x increases from 0 to 1, a/b[O] increase from 0.98366 to 1 indicating a transition of structural phase from orthorhombic to tetragonal. The increase in a/b[AO] is

attenuated and the orthorhombic structure is retained. For a given x, the heat treatment [AO] decreases a/b. This decrease increases with x. This is a sign of the reduction in the cation and anion disorders with x. When x increases from 0 to 1, T_c[O] decreases but a/b [O] increases. Then for x > 0.2, T_c [AO] and a/b[AO] increases as expected in RE123 [3].

IV. CONCLUSIONS

Our study is based on the research of the parameters which influence the structural and superconductive property in $(Y_{1-x}Sm_x)SrBaCu_3O_{6+z}$. By using two heat treatments ([O] and [AO]), we have obtained different critical temperatures in the same compound (T_c[O] ≠T_c[AO]). For each x, the a/b[O] ratio is higher than a/b[AO] ratio. Thus, the critical temperature T_c increases and a/b ratio decreases, except in the case of x≥0,2 for sample [AO], where a/b ratio increases with T_c .

The heat treatment influences the parameters a and b, the surface s, the a/b ratio and the critical temperature T_c. The variation of the parameters a, b, s and a/b influences the oxygen disorder in the basal plans (or NOC). The transfer of charge between the two coppers, Cu(2) of plane and Cu(1) of chain is effected by the insertion of oxygen in the basal plane or order/disorder oxygen on this plane, via the apical oxygen O(1). This is justified by the correlation between, the number of the holes p_{sh}, the critical temperature T_c and the inverse distance $d^{-1}[Cu(1)-Cu(2)]$ as function of x(Sm) and heat treatments in $Y_{1-x}Sm_xBaSrCu_3O_{6+z}$.

Several factors like the change of the ionic ionic size of the rare earth Sm in $YBaSrCu_3O_{6+z}$, its disorder on the site (Sr/Ba), the oxygen order of the chains or the surface, atomic distances, heat treatment and the a/b ratio, influence the critical temperature T_c by intermediary of the number of the holes in the copper $Cu(2)O_2$ plans. The parameter which governs the superconducting in our samples is the density of the holes in the $Cu(2)O_2$ plans.

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