Structure Refinement of Zn and Pr-doped Y-Ba-Cu-Oxides

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Abstract. Superconducting compounds of composition $Y_{0.9}$ $Pr_{0.1}Ba_2$ $[Cu_{1-y}Zn_y]_3O_{7-\delta}$ ($0 \leq y \leq 0.10$) have been synthesized. The structure of these materials has been studied using powder X-ray diffraction technique and refinement has been carried out by using Rietveld refinement procedure. It has been shown that all these compounds crystallize in orthorhombic structure with slight change in c parameter. Increase of parameter O(2) and decrease of parameter O(3)suggest the changes in the Cu-O2 plane of these orthorhombic materials on Zn substitution.

INTRODUCTION

The substitution with rare-earth element at the cation Y site and transition elements at Cu site of the high temperature superconductor $YBa_2Cu_3O_{7-\delta}$ (Y123) is an important method of understanding the mechanism of the occurrence of superconductivity at high temperatures. [1] All cuprate superconductors possess highly conducting two dimensional Cu-O networks .[2] The insensitivity of the superconducting properties to the rare-earth substitution is presumably due to their layered structure and the nearly complete lack of interaction between rare-earth and CuO2 sheets .[3] With this in mind the present investigation was undertaken in order to see whether there is any change in crystal structure parameters due to combined doping effect of Zn at Cu site and Pr at Y site. In particular, the attention is paid to the changes in the lattice constants as well as the atom positions in Y-Pr-Ba-Cu oxide superconductors.

EXPERIMENTAL ANALYSIS

Polycrystalline samples of $Y_{0.9}$ $Pr_{0.1}Ba_2$ $[Cu_{1-y}Zn_y]_3O_{7-\delta}$ with $0 \leq y \leq 0.10$ were synthesized by standard solid-state reaction methods using high-purity(> 99.99%) powders [4]. XRD patterns were recorded on a Rigaku X-ray Diffractometer with CuKα radiation at a scan rate of 0.200 /min with 0.020 step size in the 2θ Range between 20 and 800.The oxygen content of the samples was determined by iodometric titration which is found to be 6.67 ± 0.03. Electrical resistivity measurements were measured on Four Probe setup using silver point contacts in the temperature range 14-300K, in order to check the superconducting nature of these materials.

RESULTS AND DISCUSSION

X-ray diffraction patterns of samples of composition $Y_{0.9}$ $Pr_{0.1}Ba_2$ $[Cu_{1-y}Zn_y]_3O_{7-\delta}$ with $0 \leq y \leq 0.10$ are shown in Figure 1 . The structural parameters were refined by Fullprof program. Rietveld refined XRD profiles are shown in the same figure. The Rietveld analysis was carried out for the space group Pmmm with Y(½,½,, ½) , Pr(½,½,, ½), Ba (½,½, z) ,Cu(1)(0,0,0), Cu(2) (0, 0, z), O(1) (0, ½ , 0), O(2) (½, 0 ,z) , O(3)(0, ½, z) , O(4) (0, 0, z). Rietveld refined XRD profiles of $Y_{0.9}$ $Pr_{0.1}Ba_2$ $[Cu_{1-y}Zn_y]_3O_{7-\delta}$ with y = 0.01 is shown in Figure 2 .Results of structural analysis presented in Table 1 show although Zn with +2 valency substitutes at Cu (2) site and Pr with +3 valency at Y site the orthorhombic symmetry of Y123 system remains almost invariant. This can be easily seen by the visual

2nd International Conference on Condensed Matter and Applied Physics (ICC 2017)
AIP Conf. Proc. 1953, 120018-1–120018-4; https://doi.org/10.1063/1.5033083
Published by AIP Publishing. 978-0-7354-1648-2/$30.00

examination of the diffraction patterns given in Figure1 and comparing them with reported XRD patterns of orthorhombic Y123 structure [2].

The resistivity plot for $Y_{0.9}$ $Pr_{0.1}Ba_2$ $[Cu_{1-y}Zn_y]_3O_{7-\delta}$ with $0 \le y \le 0.10$ is shown in Figure 3 and the transition temperature are presented in Table 1. These plots clearly show that our samples are superconducting. The decrease in Tc with increase in Zn content indicates some structural change in these oxide

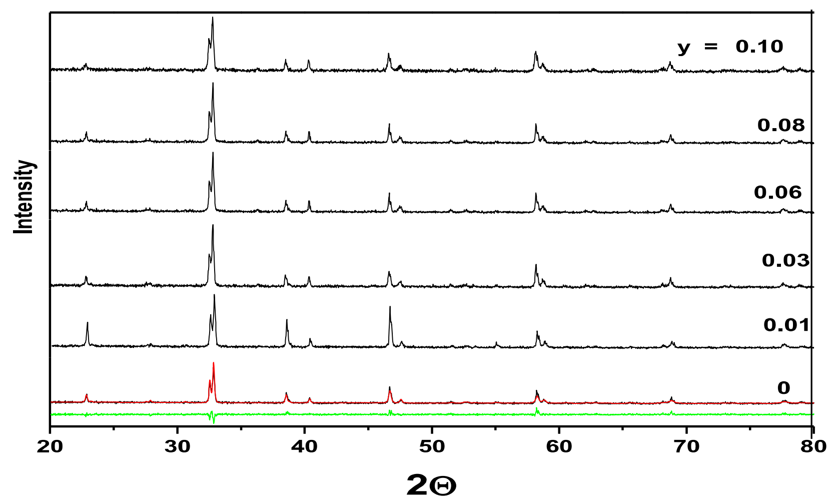

FIGURE 1 : XRD profiles of $Y_{0.9}Pr_{0.1}Ba_2[Cu_{1-y}Zn_y]_3O_{7-\delta}$ with $0 \le y \le 0.10$

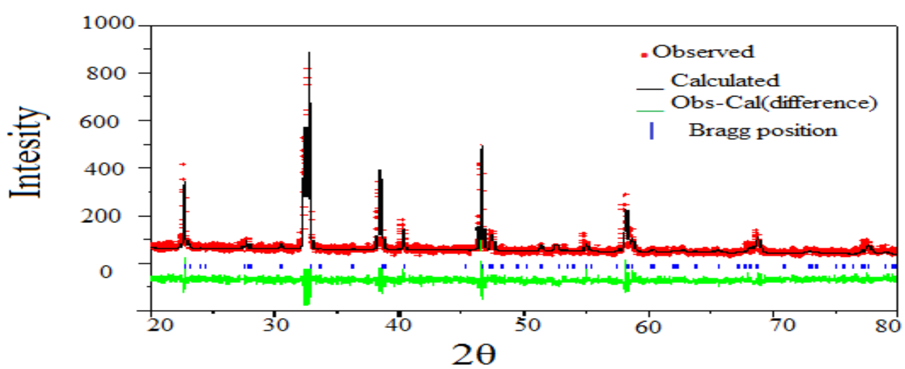

FIGURE 2 : Rietveld refined XRD profiles of $Y_{0.9}Pr_{0.1}Ba_2[Cu_{1-y}Zn_y]_3O_{7-\delta}$ with $y = 0.01$

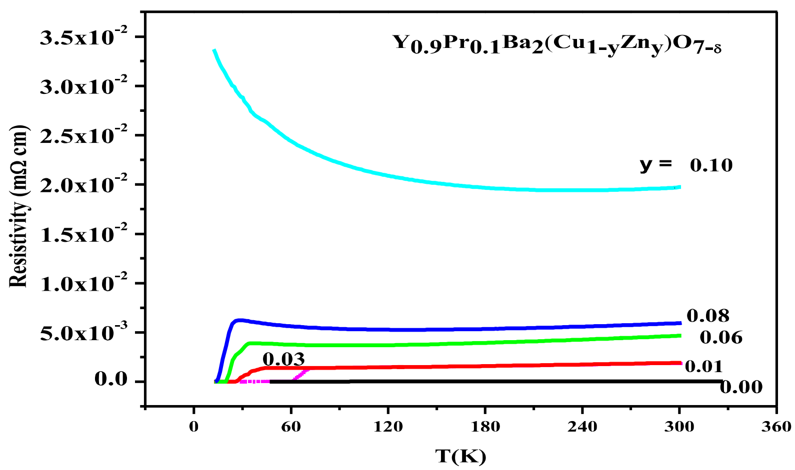

FIGURE 3: Resistivity against temperature for $Y_{1-x}Pr_xBa_2[Cu_{1-y}Zn_y]_3O_{7-\delta}$ samples with different values of Zn concentration and x =0.10

Table 1 rietveld refinement of XRD data for $Y_{0.9}Pr_{0.1}Ba_2[Cu_{1-y}Zn_y]_3O_{7-\delta}$
(The value in the parentless represents uncertainity in the last digit)

	y = 0.0	y = 0.01	y = 0.03	y = 0.06	y = 0.08	y = 0.10
z(Ba)	0.182(3)	0.182(3)	0.182(3)	0.182(3)	0.178(3)	0.178(3)
z(Cu2)/z(Zn)	0.361(2)	0.360(2)	0.361(2)	0.361(2)	0.359(2)	0.362(2)
z(O2)	0.366(4)	0.367(4)	0.396(2)	0.383(2)	0.379(2)	0.378(2)
z(O3)	0.388(1)	0.388(1)	0.355(4)	0.370(3)	0.336(5)	0.336(5)
z(O4)	0.160(2)	0.163(2)	0.159(4)	0.159(4)	0.156(4)	0.158(4)
$a(A^0)$	3.820(2)	3.820(2)	3.823(2)	3.824(2)	3.826(2)	3.827(2)
$b(A^0)$	3.884(3)	3.884(3)	3.883(3)	3.887(1)	3.888(1)	3.889(1)
$c(A^0)$	11.663(1)	11.663(1)	11.665(1)	11.658(2)	11.668(1)	11.669(1)
R_{wp}	16.0	15.0	12.6	15.4	15.6	15.0
R_{exp}	14.0	12.0	13.6	13.5	14.4	13.8
R_{Bragg}	12.67	12.91	11.4	9.96	16.27	13.99
χ^2	1.22	1.29	1.27	1.30	1.18	1.18
$T_c(K)$	77	62	26	19	13	-

Careful examination of Table 1 shows that the lattice parameters a, and b do not change much however, c parameter is slightly affected thereby slightly affecting the O(4) parameter which is responsible for keeping the structure to be orthorhombic. It is seen that that with Zn substitution the parameter O(2) increases whereas parameter O(3) decreases thereby suggesting the changes in the Cu-O2 plane of these orthorhombic materials.

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