Variation of Lattice parameters due to Cd-substitution in $(Y_{0.8}Pr_{0.2})\ Ba_2Cu_3O_{7-\delta}$ superconductor

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Abstract:
In the present communication, a study on variation in lattice parameter of unit cell of $(Y_{1-x-y}\ Pr_x\ Cd_y)\ Ba_2Cu_3O_{7-\delta}$ *superconducting polycrystalline material is presented. Atoms of Cd occupy the site Y of yttrium atoms and thus with increase of Cd as a substitute, considerable change in superconducting properties is expected. It is observed that as the Cd substitution increases, the parameters of the orthorhombic structure also increase to yield an increase in unit cell volume. The effect of this produces suppression in superconductivity which will be reported elsewhere.*

Keywords: *Variation in lattice, Cd substitution, Superconductivity*

1. Introduction

X-ray diffraction (XRD) is the most powerful and commonly used technique to investigate the structural characteristics of high-T_c superconductors. X-ray diffraction studies help to know the structural phase present in the sample and the analysis of XRD patterns give the values of unit cell parameters of the system under investigation. Knowledge about emergence and disappearance of certain Bragg reflections in the XRD patterns reflect the associated structural changes occurring due to various factors like temperature, oxygen content, substitutions, etc. in the samples. Usually, XRD studies are performed on polycrystalline samples.

A crystallographic unit cell of YBa2 Cu_3 $O_{7-\delta}$ comprises of triple layered perovskite type structure consisting of the layers of Cuo_2-BaO-CuO-BaO-CuO_2 separating two yttrium ions. For $0 < \delta < 0.6$ i.e. the oxygen content between 7.0 to 6.4, the unit cell has an orthorhombic structure with the phase group P_{mmm} containing one formula unit per unit cell [1]. The unit cell consists of two crystallographic distinct copper sites namely Cu (1) and Cu (2) in 1-D chains and 2-D planes with four-fold and five fold coordination's respectively. Oxygen atoms are named according to the distinct sites, they occupy namely O (1) and O(5) in CuO chains, O(2) and O(3) in CuO planes and O(4) in the BaO plane [2] . The yttrium atom is located in the centre of unit cell and do not have any oxygen in its plane while two Ba atoms present on both sides of the yttrium consist of oxygen in their plane and separates the CuO chains and planes.

2. Experimental

All the samples with different concentration of x and y in the system $(Y_{1-x-y}Pr_x\ Cd_y)\ Ba_2Cu_3O_{7-\delta}$ were prepared using standard solid state reaction method. The stoichiometric quantities of required constituent oxide of yittrium, Copper, Praseodymium, Cadmium and Barium Carbonate all AR grade chemicals were thoroughly dry mixed in a agate morter. After following the standard solid state reaction method, sample pellets were prepared at a pressure of 2 tonescm^2. The prepared samples with stoichiometric composition with polycrystalline structure of $(Y_{1-x-y}\ Pr_x\ Cd_y)\ Ba_2Cu_3O_{7-\delta}$ .were studied for XRD. The XRD studies were carried out using JEOL -800 DX X-ray diffractometer using Cuk_α

radiations. XRD patterns of all the samples studied obtained in the 2θ range of 20^0 to 70^0, with a step size of 0.02 and step time 1.0. Analysis of the XRD patterns was carried out using modified Gaussian functions and refined unit cell parameters calculated using the standard least squares programme are listed in table-I.

Table-1: XRD patterns using modified Gaussian functions and refined unit cell parameters

Sample (x, y)	a (A^0)	b (A^0)	c (A^0)	Ortho-rhombicity $\frac{(b-a)}{(b+a)}$ x 100%	Volume $(A^0)^3$	Density dx gm/cm^3
x = 0.0 y = 0.0	3.8301	3.8988	11.6682	0.8889	174.239	6.239
x = 0.2 y = 0.0	3.8358	3.8940	11.6766	0.7529	174.409	6.387
x = 0.2 y = 0.1	3.8376	3.8953	11.6865	0.7462	174.697	6.437
x = 0.2 y = 0.2	3.8415	3.8956	11.6819	0.6992	174.819	6.425
x = 0.2 y = 0.3	3.8471	3.8957	11.6937	0.7578	174.800	6.428

In Figure 1 and 2, a scientific representation of XRD patterns is being analysed. Modified Gaussian functions are used to fit the data, and a standard least squares program is employed to refine and calculate the unit cell parameters of a crystalline material.

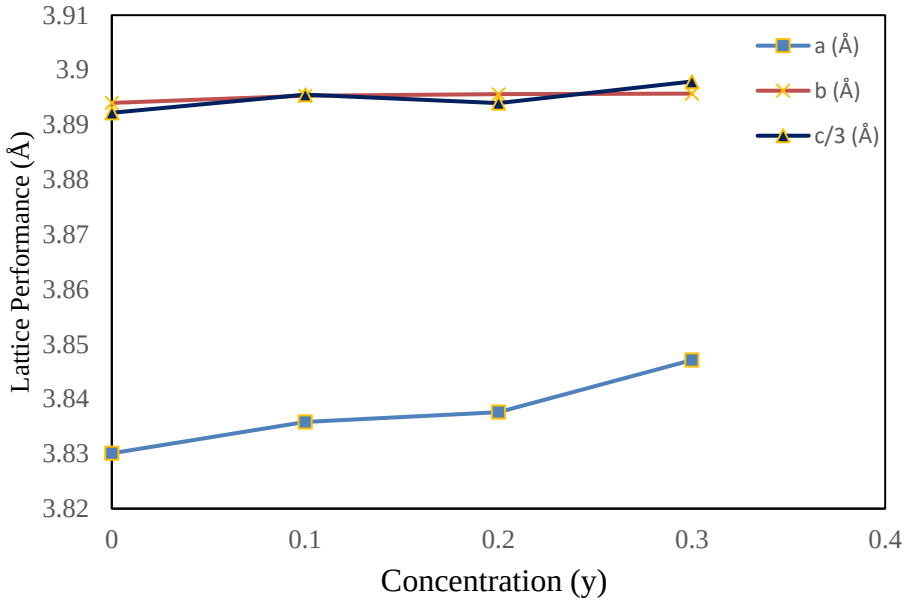

Figure 1: Plot of Lattice Performance (Å) Vs Concentration (y)

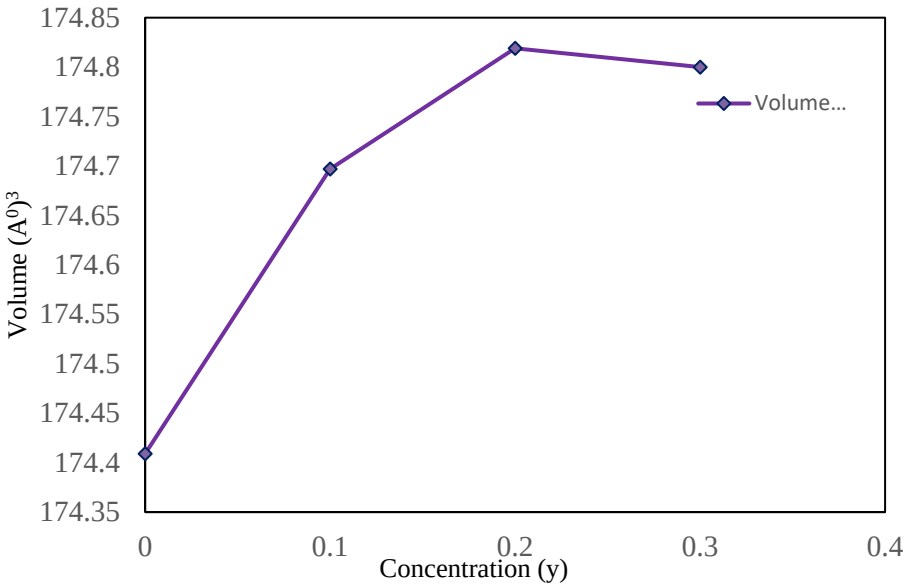

Figure 2: Plot of Volume $(A^0)^3$ Vs Concentration (y)

3. Result and Discussion

The values of the lattice parameters for (x = 0. 0, y =0.0) sample (Prestine Y-123) and (x =0.2 , y=0.0) sample ($Y_{0.8}$ $Pr_{0.2}$) $Ba_2Cu_3O_{7-\delta}$ are in good agreement with the reported data [3]. All the Pr-Cd doped samples remain orthorhombic with orthorhombic distortion very close to that of pure 123. The table also lists the values of volume and density of the samples studied.

4. Conclusion

It can be seen from the table that there is small variation in unit cell parameters with Cd substitution which displays increasing unit cell volume with increasing Cd. A comparison between the present results with the Ca-doped ($Y_{0.8-y}$ $Pr_{0.2}Ca_y$) $Ba_2Cu_3O_{7-\delta}$ system reveals the similarity in the variation of lattice parameters and volume [4].

References

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