

Research Article

Studying the Effect of Yttrium Concentration on the Structural and Superconducting Properties of YBCO Superconductors

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Abstract

High-temperature superconductors (HTS) are widely utilized in modern technological applications due to their unique properties, primarily the expulsion of magnetic fields and nearly zero electrical resistance. This study investigates the influence of varying yttrium (Y) concentrations on the structural and superconducting properties of Yttrium Barium Copper Oxide (YBCO) superconductors. Three samples with different Y concentrations (Y = 1.00, 0.90, and 0.80) were synthesized using a solid-state reaction method. The prepared samples were characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM). XRD results revealed a phase transition from orthorhombic (space group Pmmm) at higher Y concentrations (Y = 1.00 and 0.90) to tetragonal (space group P4mmm) at Y = 0.80, indicating a deterioration of superconducting properties. SEM analysis showed significant microstructural changes with Y concentration variations. The Y = 0.90 composition demonstrated an optimal balance of grain connectivity and porosity, suggesting it is suitable for high-performance superconducting applications. These findings highlight the critical role of yttrium concentration in tailoring YBCO properties for specific technological uses.

Keywords

YBCO Superconductor, Yttrium Concentration, XRD, SEM, Phase Transition, Superconducting Properties

1. Introduction

Superconductors are a class of materials known for their extraordinary property of zero electrical resistance and the expulsion of magnetic fields below a certain critical temperature, making them essential in modern scientific and technological applications [1]. Since their discovery by Heike Kamerlingh Onnes in 1911, superconductors have revolutionized fields ranging from energy systems to medical im-

aging and quantum computing [2].

Among high-temperature superconductors (HTS), Yttrium Barium Copper Oxide (YBCO) holds significant prominence due to its high critical temperature (T_c) around 92 K, which allows it to function effectively with liquid nitrogen—a more economical cooling option compared to liquid helium [3]. YBCO's superior flux pinning properties and stability under

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high magnetic fields have made it indispensable for advanced applications, such as power cables, magnetic levitation (maglev) systems, and superconducting magnetic energy storage (SMES) systems [4].

The superconducting performance of YBCO is highly sensitive to its elemental composition, particularly the ratios of yttrium, barium, copper, and oxygen. Even minor alterations in these stoichiometric ratios can lead to significant changes in critical temperature (T_c), critical current density (J_c), and grain boundary characteristics [5]. Yttrium plays a central role in stabilizing the orthorhombic structure of YBCO and influences the charge carrier concentration essential for superconductivity [6].

Motivated by the necessity to optimize the superconducting properties for practical applications, this research focuses on exploring the effect of varying yttrium concentration in YBCO compounds. Prior studies indicate that deviations in yttrium content can either enhance or degrade superconducting performance, thus making it a critical parameter for investigation [7]. The primary objective of this research is to systematically investigate how variations in yttrium concentration affect the structural, electrical, and superconducting properties of YBCO materials. The research is guided by the following key, the influence of yttrium concentration on the crystal structure of YBCO (2), the impact on critical temperature (T_c) Is there an optimal yttrium concentration that maximizes superconducting performance for high-temperature applications [15].

2. X-ray Diffraction (XRD)

X-Ray Diffraction (XRD) is a technique used to study the structure of a crystal in atomic and molecular materials by diffracting a beam of X-rays in all directions. In general, the function of the XRD tool is to identify and analyze the phase of a material, in the form of powder or solid from inorganic samples, in the form of polycrystalline and amorphous. XRD can be used for qualitative and quantitative analysis. the quantitative analysis, the data presented is including of two theta angles, peak intensity, and the amount of lattice constant [8]. For qualitative analysis, the data includes phase analysis, which can be in the form of identification of the type of phase, phase composition (percentage), crystallite size, orientation.

The YBCO samples were characterized by using X-ray diffraction technique (XRD), The phase purity and structural analysis of the composite samples were scanned through XRD (Rigaku Ultima-IV X-ray Diffractometer with $\text{CuK}\alpha$ radiation of the wavelength of 1.54 Å) with a step size of 0.02°. The Rietveld refinement analysis gives brief information about the structural parameters and variation in oxygen content of the pure sample, the refinement data are well analyzed through a software [9]. Then surface modifications of the specimens were analyzed with a resolution of 3 nm) analysis. To analyze the size distributions of grains and variation of strain in YBCO matrix. Figure 1 shows the XRD instrument structure [9, 15].

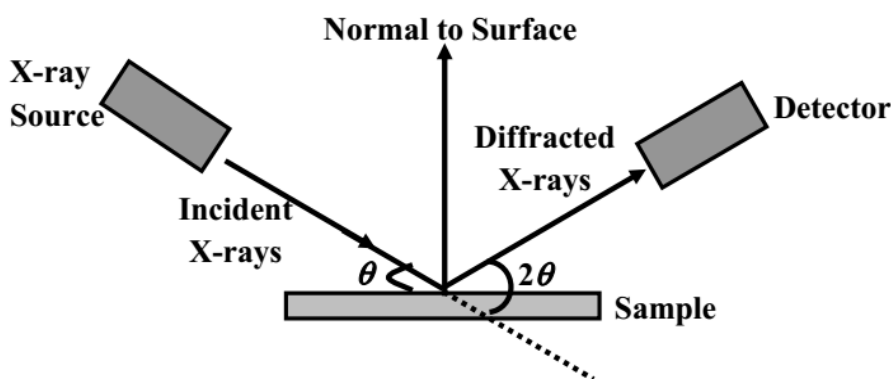


Figure 1. XRD instrument structure.

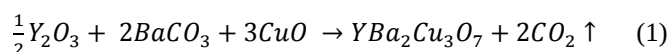
3. Materials and Methods

3.1. Materials

Yttrium oxide (Y_2O_3) – Wight powder, Barium Carbonate (BaCO_3), Copper oxide (CuO) – black powder, Diluted sulfuric acid Distilled water.

The desired superconducting compound was obtained, each of Y_2O_3 (0.151 gm), BaCO_3 (0.529 gm), CuO (0.320 gm) were considered as initial weights equivalent to 1 gm for the whole

sample. There were three samples prepared in order investigate the present of Yttrium in the compound. To increase the quantity of the sample, each of the starting materials were multiplied by 3, and as the results the new calculated weights were obtained from the below equation.



3.2. Sample Preparation

Three samples were prepared by varying the Y_2O_3 content

while maintaining constant BaCO_3 and CuO amounts:

- 1) Sample 1 ($Y = 1.00$): 0.453 g Y_2O_3 , 1.587 g BaCO_3 , 0.96 g CuO .
- 2) Sample 2 ($Y = 0.90$): 0.4077 g Y_2O_3 , 1.587 g BaCO_3 , 0.96 g CuO .
- 3) Sample 3 ($Y = 0.80$): 0.3624 g Y_2O_3 , 1.587 g BaCO_3 , 0.96 g CuO .

Samples were prepared and the above weights were achieved using a sensitive balance with atmosphere insulating glass. In the beginning, the Mortar was washed using the distilled water, and diluted sulfuric acid by 40%. The washing process has been done in sequence, first the tool was washed by using tap water, followed by immersing into the diluted sulfuric acid, then it was kept dry and washed for the second time by using the distilled water. Tools were eventually washed by acetone to guaranty the removal of any unwanted contaminants [13, 14].

Began with the first sample (100% present of Y_2O_3), the dry mix is ground with clockwise gentle movement for 30

mins, until a gray mixed powder was obtained. The powder was carefully transferred to high temperature resistance crucible, and placed into Carbolated oven for 1 hour at 850 °C. After the oven was cooled down, the black mixture was removed into the Mortar and ground with addition of acetone, for 30 minutes. Again, the mixed gray powder was placed into the oven for 5 hours at 850 °C. As final step, oven was cooled down to the room temperature, and the hard burned powder was ground for 30 minutes and taken to the analysis afterward.

Following the same above way, sample 2 and 3 were prepared with 90%, 80% in Sequence. Characterization Techniques.

XRD: Rigaku Ultima-IV X-ray Diffractometer with $\text{Cu K}\alpha$ radiation ($\lambda = 1.54 \text{ \AA}$), step size 0.02° , used for phase and structural analysis [10].

SEM: Morphological analysis to evaluate grain size, distribution, and surface features of the sintered samples [11].

4. Results and Discussion

XRD Analysis:

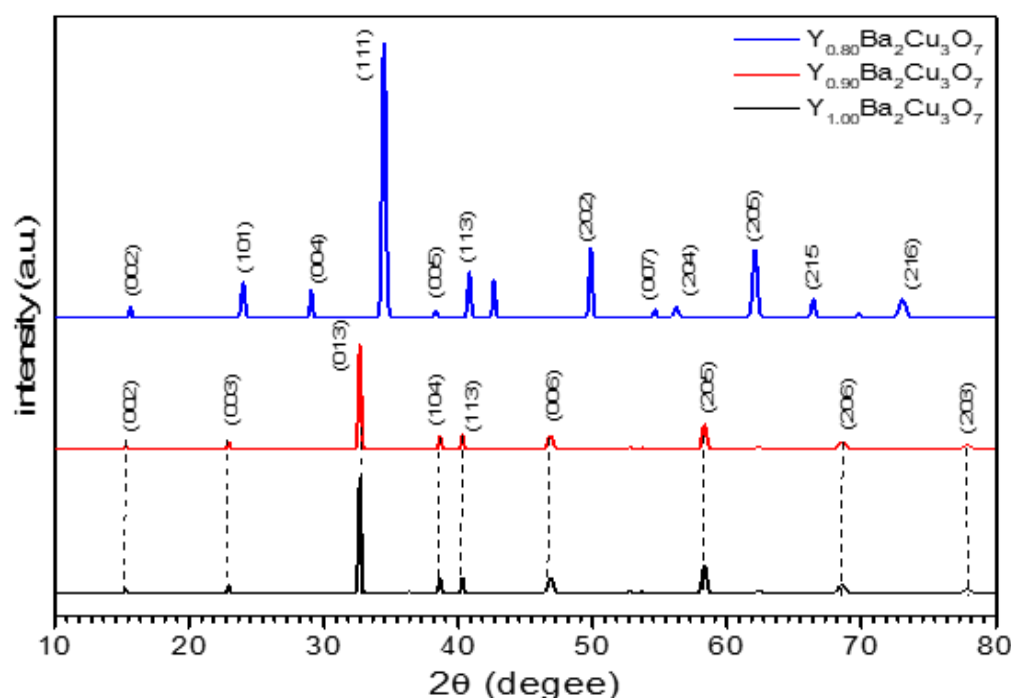


Figure 2. XRD pattern of YBCO samples with different Y content.

Table 1. Structural properties of YBCO samples with different Y content.

XRD Data	$\text{Y}_{1.00}\text{Ba}_2\text{Cu}_3\text{O}_7$	$\text{Y}_{0.90}\text{Ba}_2\text{Cu}_3\text{O}_7$	$\text{Y}_{0.80}\text{Ba}_2\text{Cu}_3\text{O}_7$
Space Group	Pmmm (47)	Pmmm (47)	P4/mmm (123)

XRD Data		$\text{Y}_{1.00}\text{Ba}_2\text{Cu}_3\text{O}_7$	$\text{Y}_{0.90}\text{Ba}_2\text{Cu}_3\text{O}_7$	$\text{Y}_{0.80}\text{Ba}_2\text{Cu}_3\text{O}_7$
Crystal System		Orthorhombic	Orthorhombic	Tetragonal
Cell Parameters (Å)	a	3.82	3.84	3.87
	b	3.89	3.89	3.87
	c	11.68	11.70	11.73
Density (g. cm^{-3})		6.33	6.32	6.21
Volume (10^6 pm^3)		173.56	174.77	175.68
d (Å)		2.461905	2.470815	2.473578
Particle size (nm)		34.13	32.73	30.87

Important structural changes of the samples exhibiting differences in Y concentration, such as 1.00, 0.90, and 0.80, have been determined by the XRD analysis of the samples, which affect the physical properties of the samples, especially the superconducting behavior. The transition from an orthorhombic to a tetragonal structure with the decrease in Y concentrations indicates the presence of oxygen deficiency in YBCO, which determines its crystallographic and functional properties.

In the samples with Y = 1.00 and Y = 0.90, the structure remains orthorhombic with the Pmmm (47) space group (JCPDS NO.01-082-0393), typical for oxygenated YBCO and superconducting. The phase transition at Y = 0.80 leads to a tetragonal structure with the P4/mmm (123) space group (JCPDS NO.01-078-1730) [10]. This structural transition is usually accompanied by oxygen loss, which destroys the Cu-O chains serving as the superconducting carriers. These results are in good accordance with previous studies showing a strong correlation between superconductivity and oxygen ordering in YBCO, and the transition to the tetragonal phase is accompanied by the deterioration of superconducting properties. Changes in the lattice parameters also support this interpretation.

A slight increase in the a and c parameters, together with unit cell volume expansion, would indicate lattice distortion due to changes in Y content. Although the b parameter does not change for Y = 1.00 and Y = 0.90, it shows a slight reduction at Y = 0.80, indicating atomic rearrangements and, consequently, some strain within the crystal lattice. The expansion may also be due to the cationic disorder or defect formation in these samples that could influence the electronic

structure and transport properties in YBCO. The average crystallite size of the prepared powders was calculated from XRD line broadening using the Debye-Scherrer equation,

$$d = \frac{K \lambda}{\beta \cos \theta} \quad (2)$$

Where λ is the wavelength of the X-ray radiation ($\text{Cu-K}\alpha=1.5406 \text{ Å}$), K is a constant taken as 0.89, β full width at half maximum height (FWHM in radian), and θ is the diffraction angle. Apart from this, there is a great crystallite size reduction as soon as the Y content decreases, from 34.13 nm at Y = 1.00 to 30.87 nm at Y = 0.80. Such reduction in crystallinity indicates an increased lattice strain and disorder, probably due to oxygen vacancies or other imperfections within the crystal lattice.

A smaller crystallite size further results in an increased density of grain boundaries that may affect charge carrier mobility and, thus, the superconducting performance of the material. From the combined structural variations, one can conclude that the superconductivity properties of YBCO are highly sensitive to changes in both the Y content and the oxygen stoichiometry. The transition into the tetragonal phase, at Y = 0.80, from the orthorhombic phase, indicates that the material becomes oxygen-deficient, which destroys the chain network of Cu-O and is unfavorable to superconductivity. The results obtained make it imperative that the exact amount of Y content and oxygen level be controlled so that the desired structural phase is retained by the material with an optimized superconducting property [12, 14].

Table 2. properties of YBCO samples. with different Y content.

Sample	Structure	Space Group	Crystallite Size (nm)	Density (g/cm^3)
Y = 1.00	Orthorhombic	Pmmm (47)	34.13	6.33
Y = 0.90	Orthorhombic	Pmmm (47)	32.73	6.32

Sample	Structure	Space Group	Crystallite Size (nm)	Density (g/cm ³)
Y = 0.80	Tetragonal	P4/mmm (123)	30.87	6.21

Notably, reduction in yttrium led to lattice distortion and reduced crystallite sizes, suggesting oxygen deficiency and impaired superconducting pathways at Y = 0.80.

5. SEM Analysis

The scanning electron microscope (SEM) is a multifunction apparatus which is also recognized as SEM analysis or SEM technique, has been used worldwide in many disciplines

which is a very developed SEM Quanta device for materials science. It can be regarded as an effective method in analysis of organic and inorganic materials in a range of nanometer to micrometer (μm) scale which is used for imaging and analyzing bulk specimens utilizing interaction between irradiated electrons and a specimen. Figure 3 below shows SEM equipment [11].

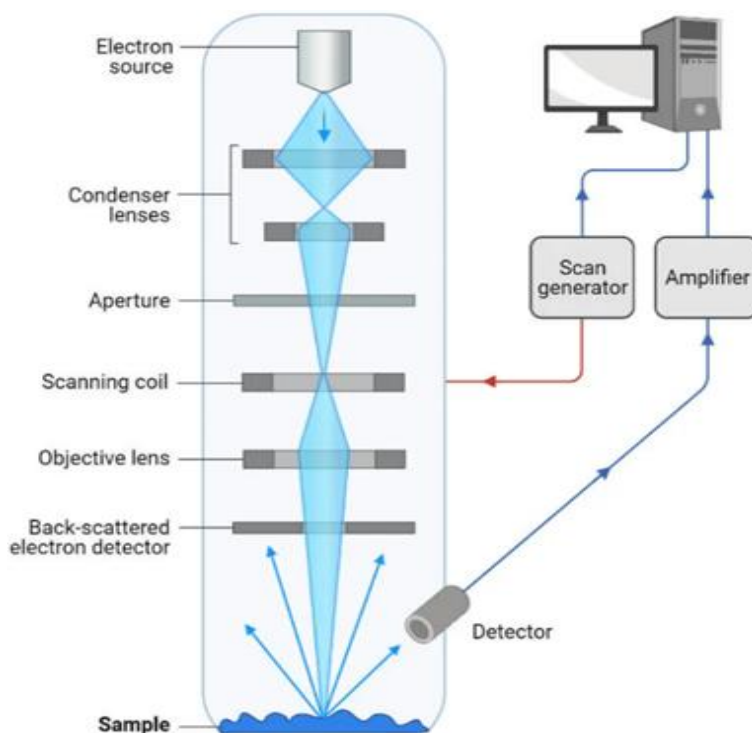


Figure 3. Schematic diagram of Scanning Electron Microscope.

SEM Micrographs:

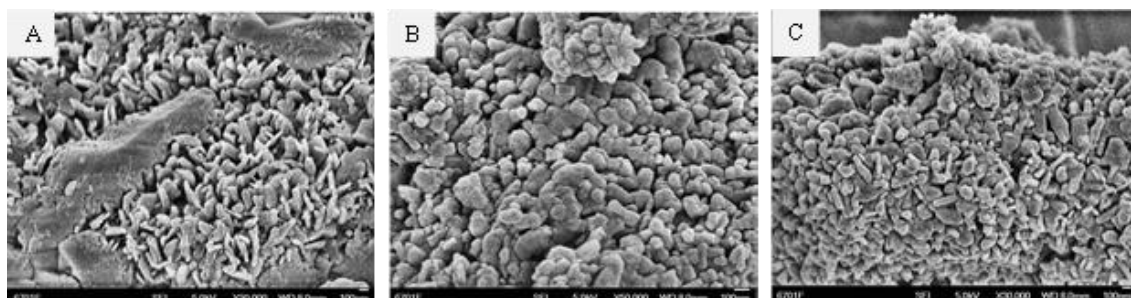


Figure 4. SEM images of (A) $\text{Y}_{1.00}\text{Ba}_2\text{Cu}_3\text{O}_7$, (B) $\text{Y}_{0.90}\text{Ba}_2\text{Cu}_3\text{O}_7$, and $\text{Y}_{0.80}\text{Ba}_2\text{Cu}_3\text{O}_7$.

Scanning electron microscopy studies were conducted on the change in morphology as yttrium varied from $Y = 1.0$, which is pure YBCO, to $Y = 0.9$ and $Y = 0.8$. A platelet-like and rod-shaped grain structure typical of the perovskite phase, along with moderate porosity, allowing good oxygen diffusion without sacrificing the necessary grain connectivity, was revealed for pure YBCO, $Y = 1.0$. This morphology is important for the establishment of effective superconducting pathways that result in stable superconducting behavior. A decrease in the yttrium content to $Y = 0.9$ resulted in a denser and more granular microstructure, which implies better grain connectivity and less porosity, hence enhanced intergranular superconducting coupling.

The microstructure became even more porous, with grain agglomeration and both elongated and rounded grains, as Y was further reduced to 0.8 . While a too-high level of porosity is unfavorable to superconducting percolation, the grain boundary non-superconductivity will enhance flux pinning and is thus useful in applications involving high magnetic fields. This may, however, be at the expense of superconducting link weakening due to the increased secondary phase formation and, hence, to performance detriments.

Overall, the $Y = 0.9$ composition had the optimum balance of grain connectivity and porosity and, hence was highly suitable for applications that demand high performance. In contrast, the $Y = 0.8$ sample displayed better flux pinning due to its phase impurities, thereby being more feasible for applications that depend on magnetic fields. Such results point to the optimization of yttrium content in synthesizing YBCO and show that careful processing conditions to engineer the microstructure can substantially enhance its superconducting properties.

6. Conclusion

XRD patterns confirmed orthorhombic structures (Pmmm, space group 47) for $Y = 1.00$ and 0.90 samples, with a transition to tetragonal (P4/mmm) for $Y = 0.80$. The results align with JCPDS cards 01-082-0393 and 01-078-1730.

The results presented in this work show that the $Y = 0.9$, $Y = 1.00$ composition had the optimum balance of grain connectivity and porosity and, hence was highly suitable for applications that demand high performance. In contrast, the $Y = 0.8$ sample displayed better flux pinning due to its phase impurities, thereby being more feasible for applications that depend on magnetic fields. Such results point to the optimization of yttrium content in synthesizing YBCO and show that careful processing conditions to engineer the microstructure can substantially enhance its superconducting properties.

SEM micrographs revealed that:

$Y = 1.00$: Platelet-like grains with moderate porosity, supporting superconductivity.

$Y = 0.90$: Denser grains with improved connectivity, op-

timal for superconducting applications.

$Y = 0.80$: Increased porosity, irregular grain morphology, indicative of compromised superconductivity but potential for magnetic field applications due to flux pinning.

7. Recommendations

YBCO (Yttrium Barium Copper Oxide) is considered an effective material for the fabrication of superconducting thin films due to its excellent superconducting properties and high critical temperature.

Abbreviations

YBCO	Yttrium Barium Copper Oxide
XRD	X-ray Diffraction
SEM	Scanning Electron Microscope

Author Contributions

Mozdlifa Bayin: Data curation, Formal Analysis, Methodology, Writing – original draft

Mahmoud Hamid Mahmoud Hilo: Supervision

Ahmed Abubaker Mohamed: Formal Analysis, Methodology, Resources, Software

Conflicts of Interest

The authors declare no conflicts of interest.

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