Article

Impact of Partial Replacement of Barium with Lanthanum on the Structural Properties of (PBCCO) System

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Abstract

This search includes the technology of solid state reactions was used to explore the impact of various pressures on the structural characteristics of (PBCCO) system . Pallets were made under various pressures, measuring 1.5 cm in thickness and (about 0.15 cm) in diameter. The pallets were sintered at an even 800 degrees Celsius for a period of 48 hours and a heating rate of (10°C / min) The structure of the materials was examined using X-ray diffraction. As per the XRD charts, each sample exhibited orthorhombic structure and we recorded the highest value of V_{ph} =0.86, 0.88 when concentrations (x=0.1,0.15) respectively . AFM (atomic force microscopy) was also used to examine the surfaces of these systems. Through it, the average diameter (nm), average roughness (Ra), and root mean square (Rg) were calculated. The results showed that the sample with the replacement ratio (0.05) had the lowest average diameter of (49.58).

Keywords: AFM , X-ray diffraction , Scherer equations , Solid state reaction technology

1. Introduction

Materials that are formed of ceramics are inorganic, non-metallic materials. They could have some crystals or all of them. The development of them is caused by heat action and subsequent cooling. In addition to strength in compression, they are brittle, hard, and weak in shearing and tension. They can withstand chemical erosion that occurs in acidic conditions. In general, ceramics are capable of withstanding very high temperatures, as those between 1000 and 1600 °C. Ceramic composites with a high dielectric constant, or High-K, are now being considered as possible candidates for use in high frequency electronics. The electronic industry will benefit from a thorough understanding of this class of materials in the planning, design, and processing of these materials . [1] Because of the important roles that crystal shape and particle size play in applications, scientists have concentrated on the production of new materials. The phases, crystal lattice properties, crystallite sizes, and crystallinity levels of the materials were ascertained using quantitative investigation. The Scherrer equation is one of the specialized methods employed in the quantitative examination. The most popular technique for determining crystallite sizes among the various technologies available is the X-ray diffractometer.. [2, 3]

2. Experimental method

specimens were made using a solid-state reaction approach, and the materials were synthesized as pure oxides in accordance with the system($PbBa_{2-x}La_xCa_2Cu_{2.9}Zn_{0.1}O_{8+\delta}$), which contained (PbO, BaO,LaO, CaO,CuO,ZnO) According to the formula, element oxides weigh an as follows :

 $PbO+(2-X)BaO+(X)LaO+2CaO+2CuO+ZnO \rightarrow PbBa_{2-x}La_{x}Ca_{2}Cu_{2.9}Zn_{0.1}O_{8+\delta}$

Then, a KERN-4-digit sensor scale was used to weigh each portion of each powder independently. where the process of grinding and mixing occurs. To achieve the best homogeneity and fine powders, the materials were first combined by hand in a gate mortar for an hour. Afterward, they were blended for two hours using an electric mixer with steel balls . Using a hydraulic press and a pressing pressure of 9 (ton/cm²) for a 2minute, the mixture powder was formed into 1.5 cm diameter cylindrical discs. To achieve the optimal and highest density, the axial pressing method was applied from two directions . Using a normal air pressure and a heating rate of 10 °C per minute, the sintering temperature of 800 °C was chosen, and the sintering time of 48 hours was observed. The samples were subsequently chilled up to room temperature at a 10 °C pace of cooling per minute in order to produce coherent samples and guarantee an optimal mechanism of atom-to-atom diffusion.

3. Results and discussion

3.1 : The XRD results are displayed in Figure (1) below . In the case of $PbBa_{2-x}La_xCa_2Cu_{2.9}Zn_{0.1}O_{8+\delta}$ compounds, the curve for intensity and 20 is between 0

and 0.2 with a 0.05 increment , all specimens' structures are orthorhombic, according to the XRD results. Additionally to their volume fractions and the Lattice parameters (a , b , c) of the respective phases, as indicated in Table1. XRD provides us with two types of information on the phases in samples . The coefficients of lattice (a , b , and c) and the X-ray chart's lattice coefficients per unit cell were calculated using a mathematical program using the following relationship [4]:

Where :(h, k, l) are Miller's coefficients .

The following mathematical relationship was used to calculate each phase's ratio [5,6] :

$$(V_{ph})\% = \frac{\sum I_o}{\sum I_1 + \sum I_2 + \sum I_{(other \, peaks)}} \times 100\% \dots \dots \dots \dots (2)$$

where I stands for the peak intensities in each phase

The Scherer equations was utilized to estimate the crystallite size values [6,7]:

$$D = \frac{k\lambda}{\beta_{hkl}\cos\theta}\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots(3)$$

where X-ray wavelength $\lambda = 1.540598$ Å , Bragg angle (θ), Scherer constant (k) = 0.9, and crystallite size (D) .



Fig (1) : Intensity as function of 20 for $PbBa_{2-x}La_xCa_2Cu_{2.9}Zn_{0.1}O_{8+\delta}$ compounds with x = 0, 0.05, 0.1, 0.15, 0.2

As shown in Figure (1), Results for high and low phases and impurities were obtained in relation to x concentrations of lanthanum La . Additionally, Table (1) lists the crystallite size values as a function of La concentration, and Figure 1 plots this relationship. The figure shows that the is crystallite size equal to 98.99(nm) at x=0, However, if the La concentration is raised above this point, the crystallite size rises as well, reaching 152.59(nm) at x=0.15. We also notice an increase in the percentage of high phases when performing the replacement process, as the high phase increased from (0.76%) for the pure sample to (0.88%) in the sample with the replacement ratio (x=0.15), which is the optimal percentage in this group, offset by a decrease in the high phase at (x=0.05), as its value was 0.75%.

Table (1) :Outcomes of the lattice parameters (a, b, and c) and the high andlow phases , value of crystallite size , crystallinity

x	a(A°)	b(A°)	c(A°)	c/a	V(A°)³	Vph(H)%	Vph(L)%	crvestallinitv%	D-Scherer(nm)
0	3 807	3 0304	11 772	3 0207	180.31	0.76	0.24	0.83	
0.05	3 902	3.3304	11 797	3.0207	181.04	0.75	0.24	0.00	105 53
0.00	3 908	3 8912	11 713	2 9974	178.09	0.75	0.23	0.73	75 75
0.15	3 915	3 9325	11 783	3 0099	181.39	0.88	0.14	0.94	152 59
0.2	3.878	3.9432	11.76	3.0326	179.83	0.78	0.22	0.7	119.45

Moreover, sintering duration is crucial for achieving phases that are thermodynamically balanced. However, to increase the number of (CuO) and (CaO) layers in the low-phase structures , a longer sintering time is needed, which led to beneficial results for the sample's high phase formation percentage[6,8]. Improvement may also be facilitated by the substitution process, it could lead to in some additional charges being transferred into the (CuO) layers and causing some copper atoms to change from the oxidation state (Cu⁺²) to the mixed state of valence (Cu⁺³) [9,10].

3.2 : AFM, or atomic force microscopy, is an excellent method for analyzing the texture and morphology of different surfaces. Knowledge of surface topography at nanometric precision has enabled research into mechanical manufacturing, tribological qualities, biological processes in motion, and mainly thin film surfaces . Compared to other microscopic approaches . The versatility of this technique allows for more in-depth examinations and assessments of the films' morphological and textural characteristics. Surface roughness was calculated using the roughness parameters (Rq) and (Ra). where the average roughness (Ra) throughout the whole measured length/area equals the mean height. The square root of the surface height distribution is known as root mean square (RMS) roughness (Rq), and it is thought to be more sensitive to significant departures from the mean line or plane than average roughness. [12]

x	Ra(nm)	Rq(nm)	Mean dimeter(nm)
0	48.29	63.4	62.34
0.05	85.79	103.3	49.58
0.1	78.89	104.8	71.77
0.15	52.82	65.39	50.58
0.2	71.67	89.68	91.1

Table (2) : average roughness (Ra) , root mean square (RMS) roughness (Rq), Mean dimeter(nm) for x=0 , 0.05 ,0.1 , 0.15 , 0.2

From table(2), the values of the (mean diameter (nm)), average roughness (Ra), and root mean square (Rq) are all affected by variations in the substitution ratio between Lathanium (La) and Barium (Ba). The sample with the replacement ratio (0.05) had the lowest mean diameter (49.58), among other characteristics. Additionally, Ra value of 85.79 nm and an Rq value of 103.3 nm . It was also

observed that when the substitution ratio between Lathanium and Barium elements increased 0.2 it leads to an increase in the mean diameter to 91.1 nm.



(x = 0.1)



0.2)

Fig (2): reveals the chart distribution and three-dimensional AFM pictures of $PbBa_{2-x}La_xCa_2Cu_{2.9}Zn_{0.1}O_{8+\delta}$

4. Conclusions

The experimental effort examined how the compound $PbBa_{2}$ $_{x}La_{x}Ca_{2}Cu_{2} _{9}Zn_{0} _{1}O_{8+\delta}$ was affected by partial substitution of lanthanum (La), Pallets were made under various pressures (5,7,9) ton/cm², measuring 1.5 cm in thickness and (about 0.15 cm) in diameter. The pallets were sintered at an even 800 degrees Celsius for a period of 48 hours and a heating rate of $(10^{\circ}C / min)$. Within the preparation conditions, for the samples, we succeeded in producing an increase in high phase. Every sample had orthorhombic structure, according to the XRD charts and the highest value of V_{ph} when $\,$ concentration (0.15) , AFM $\,$ techniques were used to examine the picture composition of the $PbBa_{2-}$ $_{x}La_{x}Ca_{2}Cu_{2,9}Zn_{0,1}O_{8+\delta}$ system with x = 0, 0.05, 0.1, 0.15, 0.2 . It shows that the less mean diameters (nm) was at (x=0.05).

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