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Annealing-Treatment Effect on the Conductivity and Porosity of BaSrTiO3 Thin Films

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Abstract: Ba0.5Sr0.5TiO3 (BST) thin films have gained significant attention due to their unique dielectric and ferroelectric properties, making them promising candidates for various electronic applications. The electrical properties of BST thin films are strongly influenced by their structural characteristics, including porosity. The phase of film and pattern characterised by XRD diffraction, and the morphology surface of film examine by FESEM technique. The dielectric constant decreased with increasing frequency, the value of dielectric constant (174,223 and 333) for 400,500, and 700ºC, respectively. The conductivity of film increased with increasing frequency (98,124 and 167 Ω).

Keywords: Electrical properties, porosity, BST, Thin Films.

1 Introduction

$BaSrTiO_3$ (BST) thin films have garnered significant interest in the field of materials science due to their unique properties and potential applications in various electronic and optoelectronic devices[1]. One crucial aspect that affects the performance and functionality of these thin films is their porosity[2]. Porosity plays a vital role in determining the electrical, optical, and mechanical properties of BST films. In this introduction, we will explore the impact of annealing temperature on the porosity of $BaSrTiO_3$ thin films[3]. Annealing is a post-deposition process that involves subjecting the thin films to specific temperatures for a defined duration, inducing structural transformations and influencing the film's properties, including its porosity[4].

Porosity in thin films refers to the presence of voids or pores within the film's microstructure. The formation and control of porosity are crucial for tailoring the film's characteristics and optimizing its performance[5]. Understanding the influence of annealing temperature on porosity provides insights into the mechanisms of pore formation, growth, and closure in BST thin films[6].

Annealing temperature plays a significant role in determining the kinetics of pore formation and growth in the films[7]. At specific annealing temperatures, the mobility and diffusion of atoms are altered, leading to changes in the formation and coalescence of pores[8]. High annealing temperatures can promote grain growth and densification, which may result in a reduction in porosity. Conversely, lower annealing temperatures may hinder pore closure, leading to higher porosity in the films[4][9].

The porosity of BST thin films has a direct impact on their electrical and optical properties. Porous films exhibit reduced dielectric constant, increased leakage current, and altered optical transmission characteristics compared to dense films[10]. Therefore, understanding and controlling the porosity through annealing temperature optimization is crucial for tailoring the electrical and optical performance of BST thin films for specific device applications[11].

The BST thin films were fabricated using a deposition technique, such as pulsed laser deposition or sputtering, followed by post-deposition annealing to optimize their crystallinity and electrical properties[12]. By carefully controlling the deposition parameters and post-annealing conditions, thin films with varying degrees of porosity were obtained.

In summary, understanding the effect of annealing temperature on the electrical properties of $BaSrTiO_3$ thin films is of paramount importance for optimizing their performance in electronic devices[13]. By comprehensively investigating the relationship between annealing temperature, crystal structure, grain size, and defect density, researchers can develop tailored fabrication processes to obtain $BaSrTiO_3$ thin films with desired electrical characteristics[14]. This knowledge will contribute to the development of advanced electronic devices with improved performance, efficiency, and reliability[15].

The findings of this study contribute to the knowledge base and provide insights into the design and fabrication of BST thin films with tailored electrical properties for future electronic and energy storage devices.

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This study aims to investigate the effect of porosity on the electrical properties of BST thin films.This study provides valuable insights into the impact of porosity on the electrical behaviour of BST thin films, facilitating the design and fabrication of high-performance thin film devices based on BST materials

2. Experimental details

BST samples were prepared using sol-gel method. Precursor powders of barium acetate, strontium acetate, were weighed in the appropriate stoichiometric ratio (Ba:Sr:Ti = 0.5:0.5:1) and thoroughly dissolved in acetic acid . The mixture was then refluxed at temperature (e.g., 110°C) for two hours to obtain the desired perovskite phase. The powders calcined at 700°C and the powers pressed into pellet form. The pellets were sintered at 1200ºC and then used as target for PLD technique. The BST pellets used as the target to deposit thin film by PLD technique.

The PLD system consists of a vacuum chamber where the deposition process takes place. The chamber is evacuated of a vacuum environment to minimize contamination and optimize BST film growth. The BST pellet is mounted in a suitable position within the chamber, facing the Si substrate. The target is topically placed on a rotating holder to ensure uniform ablation.

The substrate is carefully positioned in the chamber, facing the target, at 5 cm distance. The distance and angle between the target and substrate can affect the deposition characteristics.

The prepared BST films were subjected to annealing at different temperatures in a controlled atmosphere (e.g., air or oxygen). The annealing temperatures ranged from 400°C to 700°C.The annealing time was kept constant at 30 min for all sample.

Techniques such as X-ray diffraction, scanning electron microscopy, and LCR meter can be used for characterization of Ba0.5Sr0.5TiO3 film.

3. Results and discussion

Fig. (3) shows the XRD diffraction patterns of Ba0.5Sr0.5TiO3 annealing at different temperature. Firstly, it seen those films annealing at (400,500, 700ºC) exhibited polycrystalline phases with perovskite structure and there is no evidence intermediate phases appeared. It is clear that implies Sr^{+2} ions have entered the unit cell maintaining the perovskite structure of solid solution.

The XRD pattern shows many peaks Correspond to (100), (110), (111), (200), (210), (211) and (220) planes. These peaks are related to cubic BST phase, and the peaks perfectly match with pdf card no. (00-039-1395), with P3mm space group and lattice constant a=3.965A. The intensity of the film increased with increasing annealing temperature, which changes the crystal size, stress, and density of the film with high annealing temperatures.

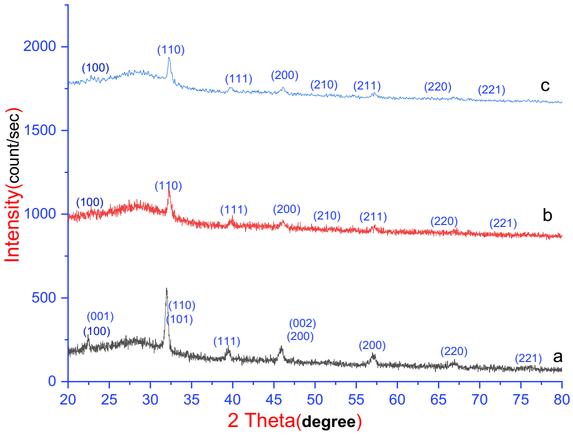

Fig. 1: XRD pattern of Ba0.5Sr0.5TiO3 Thin films with different annealing temperatures

Annealing temperature, also known as thermal treatment, is performed to improve the crystallinity and optimize the film properties. The annealing temperature directly affects the surface morphology of the BST films. It’s important to note that effects of annealing temperature on BST film morphology can vary depending on the specific deposition technique, film thickness, composition and other process parameters. Therefore, it is recommended to conduct experimental studies and optimize the annealing conditions to achieve the desired surface morphology for a particular application. Annealing temperature plays a crucial role in determining the surface morphology of barium strontium titanante(BST) films. When BST films are deposited onto a substrate, they are typically amorphous or possess a polycrystalline structure.

Annealing at elevated temperature promotes grain growth in the BST films. As the temperature increases, the atomic diffusion within the film become more active, allowing the atoms to rearrange and form larger crystalline grains. This results in a smoother surface with larger grain sizes. Higher temperature provided sufficient energy for the atoms to rearrange into a more ordered lattice structure, resulting in improved crystallinity and smother.

The annealing temperature influence the porosity of BST films. Higher annealing temperature can lead to denser films with reduced porosity. The density of film increased with increasing annealing temperature.

The results revealed that the porosity of the BST thin films significantly influenced their electrical properties. Higher levels of porosity generally led to decreased dielectric constant and increased dielectric loss due to the presence of air-filled voids or defects within the film structure.

Additionally, the porosity affected the leakage current, with higher porosity often resulting in increased current leakage. The presence of porosity also influenced the ferroelectric properties, such as remnant polarization and coercive field, thereby affecting the overall performance of BST thin films in ferroelectric-based device.

Understanding the relationship between porosity and electrical properties is crucial for the optimization of BST thin films for various applications, including capacitors, tuneable microwave devices, and non-volatile memory.

The dielectric constant and dielectric loss factor of BST depended on the physical properties and the fabrication process of BST thin films. The effect of degree crystallization on dielectric properties, there was an increase in dielectric constant with increasing annealing temperature due to better crystallinity and increase in grain size with a rise annealing temperature.

The variation in the value of the dielectric constant has been carried out at diverse temperature attributed to the grain size, crystallinity, and porosity of BST thin film. At lower annealing temperature poor crystallinity and smaller grain size of the samples induced the dielectric constant (ε) reduction.

The frequency dependence of dielectric properties in Ba0.5Sr0.5TiO3 annealing at various temperature, illustrated that the dielectric constant of Ba0.5Sr0.5TiO3 annealed at (400,500,700ºC) decrease as frequency increase attributed to different types of polarization mechanisms. Space charge polarization and dipole polarization gradually cannot catch up with change of electric field as frequency increases, which make dielectric constant decrease.

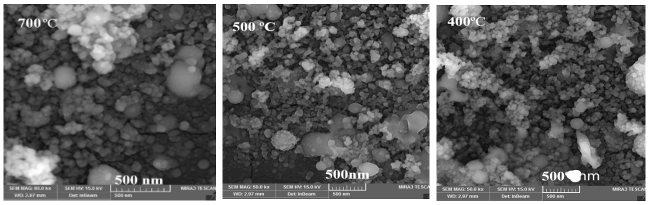

Fig. 2: the Images of FESEM for Ba0.5Sr0.5TiO3 Thin films with different annealing temperatures

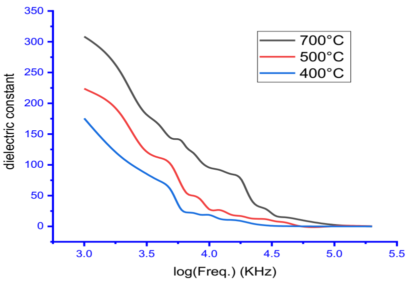

Fig. 3: the dielectric constant plotted vs frequency with different temperature

Table 1: Density and porosity with different annealing temperatures

"Sample"	400 ºC	500 ºC	700 ºC
Geometrical density (g/cm^3)	**4.12**	**4.34**	**4.78**
Theoretical Density (g/cm^3)	**5.83**	**5.74**	**5.66**
Relative density %)	**72.78**	**73.67**	**81.56**
Porosity	**27.22**	**26.33**	**18.44**

The results revealed that the porosity of BST thin films has a significant impact on their electrical properties. Higher porosity was found to decrease the dielectric constant due to the presence of air or voids within the film structure. Moreover, increased porosity resulted in a higher leakage current density, mainly attributed to enhanced charge trapping and conduction through the porous network. Additionally, the tunability of BST thin films was also affected, with higher porosity leading to a reduced tunability response.

The figure () shows the relationship between conductivity and frequency in BST thin film can be describe using the complex dielectric constant, which consist of a real part (ε) and an imaginary part (ε"). The real part represents the resistive response of the material, while the imaginary part represents the resistive response.

The conductivity (σ) can be obtained from the imaginary part of the dielectric constant using the equation:

$$\sigma = \omega\varepsilon_0\varepsilon'' \qquad (1)$$

where ω is the angular frequency (ω = 2πf) and ε_0 is the permittivity of free space.

It is important to note that the specific relationship between conductivity and frequency for BST thin films can vary depending on the film deposition method, processing conditions, and specific composition of the film.

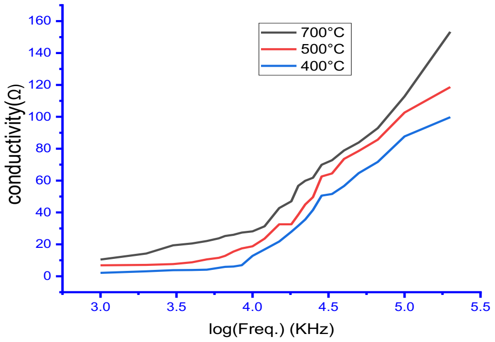

Fig. 4: the conductivity vs the frequency with different temperatures

4. Conclusion

In conclusion, investigating the effect of annealing temperature on the porosity of $BaSrTiO_3$ thin films is essential for understanding and controlling the film's microstructure and optimizing its properties. By systematically exploring the relationship between annealing temperature, pore formation, growth, and closure, researchers can develop strategies to tailor the porosity of BST thin films to meet the requirements of various electronic and optoelectronic applications. The phase of film and pattern characterised by XRD diffraction, and the morphology surface of film examine by FESEM technique. The dielectric constant decreased with increasing frequency, the value of dielectric constant (174,223 and 333) for 400,500, and 700ºC, respectively. The conductivity of film increased with increasing frequency (98,124 and 167 Ω).

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Conflict of Interest

“The authors declare that they have no conflict of interest, the project has no funding”.

Availability of data materials:

Data will not be shared because these data help study the correct choice of correct form for suitable applications.

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