The effect of ionic radius carbon dot on Ti^{4+} in lattice parameters of $Ba_{0.2}Sr_{0.8}TiO_3$ thin films

Ahmad Ripai[1,2*], *Aep* Setiawan[1,3], *W.D.* Laksanawati[1,4], *Amrullah* Kamaruddin[1,5], *Noviyan* Darmawan[6], *Johan* Iskandar[7], and Irzaman[8]

[1]Doctoral Program, Department of Physics, IPB University, Bogor, Indonesia
[2]Research Center for Climate and Atmosphere, National Research and Innovation Agency (BRIN), Bandung, Indonesia
[3]Computer Engineering Technology, IPB University Vocational School, Bogor, Indonesia
[4]Physics Education, Universitas Muhammadiyah Prof. DR. HAMKA, Jakarta, Indonesia
[5]Research Center for Sustainable Production System and Life Cycle Assessment, National Research and Innovation Agency (BRIN), Tangerang Selatan, Indonesia
[6]Department of Chemistry, Faculty of Mathematics and Natural Sciences, IPB University, Bogor, Indonesia
[7]Organic Electronics Research Center, Ming Chi University of Technology, New Taipei City, 243303, Taiwan
[8]Department of Physics, Faculty of Mathematics and Natural Sciences, IPB University, Bogor, Indonesia

Abstract. Barium Strontium Titanate ($Ba_{0.2}Sr_{0.8}TiO_3$) thin films doped with carbon dots at varying concentrations (0%, 2%, 4%, and 6%) were successfully synthesized using the Chemical Solution Deposition (CSD) method. The films were deposited on p-type (100) silicon substrates via spin coating at 8000 rpm, followed by annealing at 850 °C for 8 hours. Structural characterization using X-ray Diffraction (XRD) confirmed a cubic lattice structure for all samples, with lattice parameters (a = b = c) measured as 3.306 Å, 3.324 Å, 3.336 Å, and 3.311 Å for the 0%, 2%, 4%, and 6% doping levels. The observed increase in lattice parameters with higher carbon dot concentrations is attributed to the larger ionic radius of carbon dots (10 Å) compared to Ti^{4+} (0.61 Å). These results indicate that carbon dot incorporation modulates the structural properties of $Ba_{0.2}Sr_{0.8}TiO_3$ films, which could have significant implications for their functional applications.

1 Introduction

$Ba_{0.2}Sr_{0.8}TiO_3$ (BST) perovskite materials have garnered significant attention due to their versatile properties, making them ideal for various electronic applications such as ceramic capacitors, memory devices, and temperature sensors [1]. The dielectric properties of BST are strongly influenced by its crystal composition and structural configuration [2]. Studies have shown that altering the ionic structure of perovskite materials can significantly modify their physical and chemical properties, enabling customized material design [3].

* Corresponding author: ahmadripai@apps.ipb.ac.id

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One approach to enhance the performance of BST materials is through the substitution of titanium ions (Ti^{4+}) with innovative materials such as carbon dots. Carbon dots, which possess varying ionic radii, can induce strain effects on the crystal lattice [4]. Studies have indicated that substituting ions with radii larger than Ti^{4+} can increase lattice distortion, potentially enhancing the material's properties for specific applications [5]. Furthermore, the incorporation of nanomaterials like carbon dots has been shown to influence lattice parameters and improve the phase stability of the material [6].

The influence of ionic radius substitution on BST lattice parameters is a critical area of study, given the material's widespread use in electronic devices [7]. Experimental studies have demonstrated that variations in ionic radius can directly alter the dielectric and optical properties of perovskite materials [8]. Moreover, structural changes induced by ionic substitution are closely linked to the performance and reliability of perovskite-based devices [9].

In this study, we explore the effects of carbon dot doping on the lattice parameters of BST thin films through experimental methods. The primary objective is to examine how variations in the ionic radius of carbon dots impact the crystal structure of BST, building on findings from prior research [10]. The outcomes of this work are anticipated to advance the development of functional materials for sensor and electronic applications [11].

Doping, defined as the introduction of foreign elements into a material, plays a significant role in modifying its structural properties [12]. The impact of doping on the material's lattice structure depends on the ionic radius of the dopant. For instance, doping with ions of larger radii typically causes a shift in diffraction peaks to smaller angles (to the left), as shown in Figure 1. Conversely, doping with ions of smaller radii causes the peaks to shift to larger angles (to the right) compared to the non-doped material [13]. These changes provide valuable insights into the material's structural behavior and its potential applications.

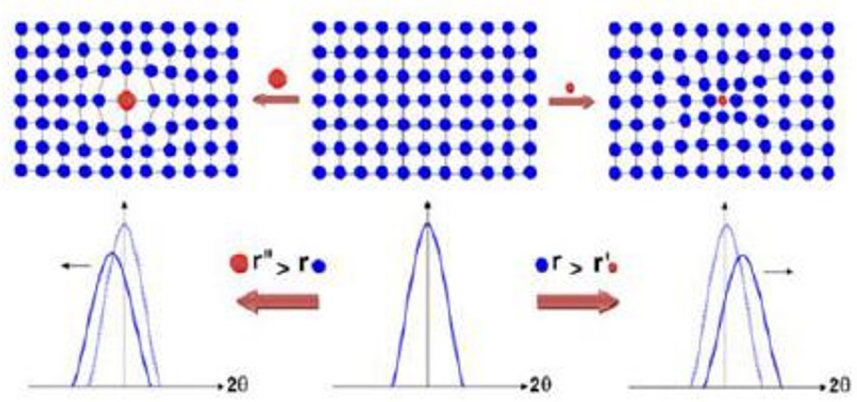

Fig. 1. Influence of ionic radius size on doping [52].

2 Research methods

2.1 Thin film synthesis

Thin films of $Ba_{0.2}Sr_{0.8}TiO_3$ were synthesized using the chemical solution deposition (CSD) method. The precursor solution was prepared by dissolving $Ba(NO_3)_2$, $Sr(NO_3)_2$, and TiO_2 in an ethanol solvent, with varying concentrations of carbon dots (0%, 2%, 4%, and 6%). The deposition process was performed on a cleaned glass substrate using the spin-coating

technique. The substrate was rotated at 8000 rpm for 30 seconds, followed by a 60-second break, repeated three times. After deposition, the samples were placed in an insulated box and annealed in a Nabertherm furnace at 850 °C [14].

2.2 Material characterization

X-ray Diffraction (XRD) was employed to determine the lattice parameters and crystal structure of the synthesized materials. XRD is a well-established technique used to analyze crystalline solid materials. This method identifies the crystalline phase by determining lattice structure parameters and estimating particle size. The X-rays generated by the instrument result from the interaction between an electron beam and atomic shell electrons. When X-rays interact with a material, three phenomena may occur: absorption, diffraction, and fluorescence [15]. XRD characterization was used to compare the crystal structures of undoped and carbon dot-doped materials.

3 Results and discussion

3.1 Synthesis and lattice parameter analysis

$Ba_{0.2}Sr_{0.8}TiO_3$ (BST) thin films were successfully synthesized with carbon dot (CD) concentrations of 0%, 2%, 4%, and 6%. XRD analysis revealed the following lattice parameter values: 3.306 Å for 0% CD, 3.324 Å for 2% CD, 3.336 Å for 4% CD, and 3.311 Å for 6% CD. These results demonstrate that the addition of carbon dots increases the lattice parameter from 0% to 4% CD concentration, while a decrease is observed at 6% CD.

3.2 Effect of carbon dot addition on lattice parameters

The incorporation of carbon dots (CD) into the BST structure influences its crystal properties through the partial replacement of Ti^{4+} ions, which have an ionic radius of 0.605 Å in octahedral coordination. Carbon dots, with their larger size due to nano composition and surface functional groups, induce lattice strain. At low CD concentrations (0% to 4%), the lattice parameters increase, primarily due to the substitution of Ti^{4+} ions, which alters the Ti–O bond interactions within the perovskite structure. Additionally, the carbon functional groups on CD generate lattice stresses, further promoting crystal structure expansion. However, at a higher CD concentration of 6%, the lattice parameter decreases to 3.311 Å. This reduction can be attributed to two factors: (1) substitution saturation, where excess CD introduces lattice defects such as oxygen vacancies or structural dislocations, reducing lattice regularity; and (2) CD aggregation, which increases the effective particle size and disrupts homogeneous dispersion, leading to compressive strains that contract the lattice structure.

3.3 Relationship between lattice parameters and material properties

Changes in lattice parameters affect the physical and electronic properties of BST, including dielectric, piezoelectric, and material response to electric fields Improvement of lattice parameters at a concentration of 4% CD, the maximum lattice parameter value of 3.336 A indicates an increase in the inter-ion distance which can improve the mobility of ions in the material, favoring higher dielectric properties. A decrease in grid parameters at a concentration of 6%, the grid parameter value of 3,311 A indicates grid defects and decreased crystal regularity, which can reduce material performance in sensor or capacitor applications.

3.4 Crystal structure analysis via XRD

The incorporation of carbon dot (CD) doping into the $Ba_{0.2}Sr_{0.8}TiO_3$ (BST) thin film structure induces significant changes in the crystal structure, as observed through XRD analysis (Figure 2). The doping process involves the partial replacement of Ti^{4+} ions in the perovskite lattice, where the larger ionic radius of carbon dots compared to Ti^{4+} (0.605 Å) generates lattice strain. This substitution increases the interplanar distances (lattice parameters) due to the pressure exerted by the larger dopant ions. In the XRD diffraction patterns (Figure 2), this expansion is evidenced by a shift in the diffraction peak to smaller 2θ values, indicating a leftward peak shift.

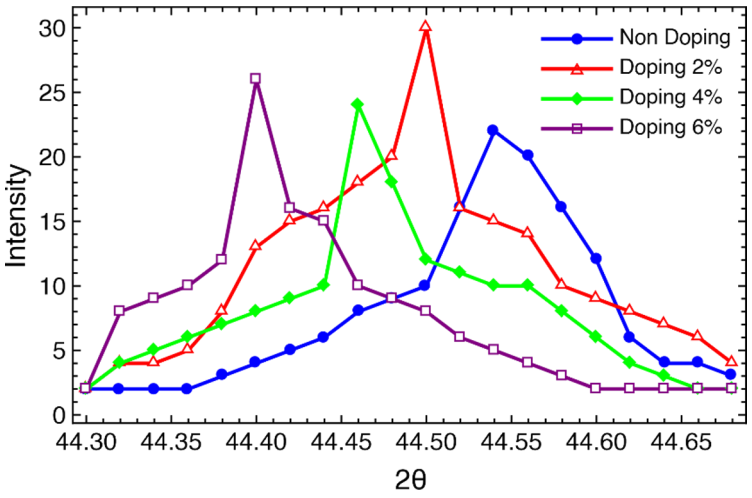

Fig. 2. Graph of the Influence of Ion Radius Size on Doping.

At low CD concentrations (2%), the diffraction peak begins to shift leftward compared to the undoped sample, suggesting lattice expansion caused by the increased spacing between crystal planes. This effect is further amplified at a 4% CD concentration, where the peak shift becomes more pronounced, reflecting a more significant expansion of the lattice parameters. The larger size of carbon dots, combined with their surface functional groups, contributes to this lattice strain.

However, at higher CD concentrations (6%), the leftward peak shift becomes less pronounced or stagnates. This can be attributed to the saturation of Ti^{4+} ion substitution, where not all lattice sites are optimally replaced. Additionally, high CD concentrations may lead to aggregation of carbon dots or the formation of structural defects, such as oxygen vacancies. These factors reduce the homogeneity of dopant distribution and introduce compressive stresses, counteracting the lattice expansion observed at lower concentrations.

In summary, the addition of carbon dots with a larger ionic radius significantly influences the lattice parameters and XRD diffraction patterns of BST. The leftward shift of the diffraction peak at low to intermediate CD concentrations confirms lattice expansion. However, at higher concentrations, factors such as substitution saturation and lattice defects must be considered, as they can compromise the stability of the crystal structure. These findings provide valuable insights for optimizing doping strategies in perovskite-based materials like BST.

4 Conclusion

The incorporation of carbon dots (CD) as dopants in $Ba_{0.2}Sr_{0.8}TiO_3$ (BST) thin films significantly influences the lattice parameters and XRD diffraction patterns. Analysis revealed that CD doping at concentrations of 2% and 4% increased the lattice parameters to 3.324 Å and 3.336 Å, respectively, compared to the undoped sample (3.306 Å). This expansion is attributed to the substitution of Ti^{4+} ions by carbon dots, which have a larger ionic radius, thereby increasing the interplanar distances within the BST perovskite structure. The leftward shift in the XRD diffraction peaks (smaller 2θ values) further confirms the lattice expansion induced by CD doping. However, at a higher CD concentration of 6%, the lattice parameter decreased to 3.311 Å. This reduction is likely caused by the saturation of Ti^{4+} ion substitution, the formation of lattice defects such as oxygen vacancies, and the aggregation of carbon dots at high concentrations. These factors introduce compressive strains, as evidenced by the slight rightward shift in the XRD diffraction peaks (larger 2θ values). In summary, CD doping at concentrations up to 4% effectively enhances the lattice parameters, as indicated by the leftward shift in diffraction peaks and the expansion of the crystal structure. However, overdoping at 6% should be avoided, as it can lead to structural defects that compromise lattice regularity. This study highlights the importance of optimizing doping concentrations to maximize the performance of BST-based materials, particularly for applications in sensors and electronic devices.

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