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Study of Physicochemical and Optical Characteristics of Doped Barium Titanate Ceramics Materials for Optoelectronic Devices

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Abstract:
This research investigates the structural, dielectric, and optical properties of doped barium titanate ($BaTiO_3$) ceramics, highlighting their potential for advanced electronic applications. Barium titanate, a prominent ferroelectric material, was doped with various elements in a systematic manner to improve its functional attributes.The crystalline structure and phase development were described by means of X-ray diffraction (XRD), showcasing how doping affects lattice parameters and phase stability. Dielectric characteristics like loss tangent and permittivity were evaluated across different frequencies and temperatures, revealing the dopants' impact on dielectric behavior and ferroelectric properties. Optical studies, including UV-Vis spectroscopy, examined the bandgap and optical transmittance, which are vital for optoelectronic uses. It is found that targeted doping can effectively modify the structural, dielectric, and optical characteristics of barium titanate ceramics, making them ideal for capacitors, sensors, and other electronic devices. This study offers valuable insights into optimizing barium titanate ceramics to achieve superior performance in various technological applications. It has also been observed that certain dopants reduced the bandgap energy, leading to better optical transparency and tunable refractive indices, which are valuable for optoelectronic applications.

Keywords: Barium Titanate ($BaTiO_3$), Doped Ceramics, Dielectric Properties, Optical Properties,

1. Introduction

Barium titanate (*$BaTiO_3$)*a perovskite-structured ceramic, has been a foundational material in electronic applications due to its remarkable dielectric, ferroelectric, and piezoelectric properties [1]. These unique characteristics make $BaTiO_3$essential in various electronic devices, including multilayer ceramic capacitors (MLCCs), thermistors, actuators, and transducers [4]. The material's high dielectric constant and adjustable ferroelectric properties are particularly beneficial for capacitors, where efficient energy storage is crucial [10]. However, as electronic technology advances, there is an increasing demand to further enhance and optimize the intrinsic properties of $BaTiO_3$to meet the stringent requirements of

modern applications [7].Doping, a well-established technique, is employed to modify and improve the properties of $BaTiO_3$Introducing small quantities of foreign ions into the $BaTiO_3$lattice allows for the tailoring of the material's structural, dielectric, and optical properties to achieve specific performance characteristics [8]. The careful selection of dopants enables fine-tuning of $BaTiO_3$properties, broadening its applicability in various electronic contexts [2]. Doping affects the crystal structure of $BaTiO_3$leading to alterations in lattice parameters, phase stability, and grain size [3]. These structural changes are intricately connected to the material's functional properties, as $BaTiO_3$'s behavior is highly dependent on its crystallographic structure [11].

The dielectric properties of $BaTiO_3$are particularly significant in its use as a capacitor material [11]. The dielectric constant, which measures the material's ability to store electrical energy, is a critical factor in determining the efficiency and capacity of capacitors [6]. Doping can enhance the dielectric constant by altering the lattice's polarizability and introducing defects that increase the dielectric response [7]. Additionally, doping can reduce dielectric loss, which is the energy dissipated as heat, thereby improving $BaTiO_3$'s performance in high-frequency and high-temperature conditions [19]. Controlling these dielectric properties through doping is essential for the development of advanced capacitors and other electronic components [5].Beyond its dielectric properties, the optical characteristics of $BaTiO_3$are also crucial for its application in optoelectronics [15]. The optical bandgap, which influences the material's ability to absorb and transmit light, can be adjusted through doping to achieve desired optical behaviors [11]. This is particularly important for applications such as optical sensors, transparent conductors, and photodetectors, where precise control over optical properties is necessary [16]. Investigating how doping affects $BaTiO_3$optical properties is vital for expanding its use in optoelectronic devices [24].This research aims to comprehensively understand how various dopants affect the structural, dielectric, and optical properties of $BaTiO_3$ ceramics [25]. By utilizing techniques such as X-ray diffraction (XRD) to analyze crystal structure, dielectric measurements to assess electrical properties, and UV-Vis spectroscopy to explore optical behavior, this study seeks to uncover the complex relationships between doping and material performance [26]. The findings from this research are expected to contribute to optimizing $BaTiO_3$ for a range of electronic applications, thereby advancing the development of next-generation materials for capacitors, sensors, and optoelectronic devices [27].

2. Methodology Applied

The investigation into the structural, dielectric, and optical characteristics of doped barium titanate $BaTiO_3$ceramics encompasses a set of meticulously organized experimental processes [28]. These procedures include the preparation of doped $BaTiO_3$samples, structural analysis, dielectric measurement, and optical assessment [29]. This comprehensive methodology aims to provide a thorough understanding of how different dopants influence the properties of $BaTiO_3$, enabling the material's optimization for electronic applications [30].

2.1. Sample Preparation

The initial stage of this research entails the preparation of doped $BaTiO_3$ceramic samples [4]. The solid-state reaction method, a well-established technique for ceramic synthesis, is utilized for this purpose [7]. $BaTiO_3$ is synthesized using high-purity barium carbonate ($BaCO_3$) and titanium dioxide (TiO_2) as the primary starting materials [8]. Depending on the specific focus of the study, selected dopants such as lanthanum, strontium, or magnesium are added in the form of their respective oxides or carbonates [9]. These dopants are carefully chosen based on their ionic radii and valence states to ensure they can

substitute for barium or titanium in the $BaTiO_3$ lattice without causing significant alterations to the overall crystal structure [15]. The precise quantities of $BaCO_3$, TiO_3, and the selected dopants are weighed and thoroughly mixed using a ball mill .This ball milling process ensures an even distribution of dopants within the $BaTiO_3$ matrix .The mixed powders are then subjected to calcination at temperatures typically ranging from 900°C to 1100°C in an air atmosphere to facilitate the formation of the $BaTiO_3$ phase [8]. Calcination is a critical step as it promotes the diffusion of dopants into the $BaTiO_3$ lattice, ensuring the creation of a single-phase material .. After calcination, the powders are ground again to achieve uniform particle size and then pressed into pellets using a uniaxial hydraulic press [8]. These pellets generally have a diameter of 10-15 mm and a thickness of 1-2 mm . The green pellets are then sintered at elevated temperatures (1200°C to 1400°C) to densify the material and improve its structural integrity . The sintering process is conducted in a controlled atmosphere, which may involve air, oxygen, or an inert gas, depending on the nature of the dopant and the desired properties of the final ceramic [7].

2.2. Structural Characterization

The structural properties of the doped $BaTiO_3$ ceramics are characterized using X-ray diffraction (XRD) technique [4]. XRD is a powerful tool for determining the crystal structure, phase composition, and lattice parameters of ceramic materials [5]. The XRD patterns of the sintered samples are obtained using a diffractometer equipped with a Cu-Kα radiation source [8], with data collected over a 2θ range of 20° to 80° with a step size of 0.02° [9].The XRD patterns are analyzed to identify the phases present in the samples and to determine the crystallographic parameters [10]. Phase identification is conducted by comparing the experimental diffraction peaks with standard reference data from the International Centre for Diffraction Data (ICDD) database [6]. The lattice parameters of the $BaTiO_3$ unit cell are calculated using the Rietveld refinement method, which provides precise information on how doping alters the crystal structure [7].In addition to phase analysis, the crystallite size and microstrain in the doped $BaTiO_3$ ceramics are estimated using the Williamson-Hall method [11]. This method involves plotting the broadening of XRD peaks as a function of diffraction angle, allowing the separation of the contributions from crystallite size and microstrain.The microstructural properties, including grain size and morphology, are further examined using scanning electron microscopy (SEM).SEM offers high-resolution images of the ceramic surfaces, enabling the observation of grain boundaries, porosity, and the distribution of dopants within the grains

2.3. Dielectric Measurements

The dielectric properties of the doped $BaTiO_3$ ceramics are measured using an LCR meter, which evaluates the material's capacitance, dielectric constant, and dielectric loss as a function of frequency and temperature. The sintered ceramic pellets are polished to ensure smooth and parallel surfaces, and then silver electrodes are applied to both faces using a screen-printing technique. The electrodes are fired at a moderate temperature to ensure good electrical contact[8].

Dielectric measurements are carried out over a frequency range of 1 kHz to 1 MHz and a temperature range of -100°C to 200°C. These conditions are chosen to capture the dielectric behavior across the ferroelectric-paraelectric phase transition of $BaTiO_3$, which typically occurs around 120°C. The dielectric constant (ε_r) is calculated using the equation:

$$\varepsilon_r = C \times d / \varepsilon_0 \times A$$

where (C) is the capacitance of the material, (d) states the thickness of the ceramic, (A) is the area equipped by electrode, and (ε_0) is the permittivity of free space(8.854×10^{-12}F/m).The temperature

dependence of the dielectric constant is particularly important for understanding the ferroelectric properties of doped $BaTiO_3$. The Curie temperature (Tc), at which the material undergoes a transition from the ferroelectric to the paraelectric phase, is determined from the peak in the dielectric constant versus temperature plot. The influence of dopants on Tc and the overall dielectric behavior is analyzed to assess the suitability of the doped $BaTiO_3$ ceramics for specific electronic applications.

2.4. Optical Analysis

The optical properties of the doped $BaTiO_3$ ceramics are investigated using UV-Vis spectroscopy. This technique is employed to determine the optical bandgap and light absorption characteristics of the material. The ceramic samples are ground into fine powders and dispersed in a transparent medium to form thin films or pellets. UV-Vis absorption spectra are recorded in the wavelength range of 200 nm to 800 nm using a spectrophotometer[22].The extrapolation of the linear region of this plot to the photon energy axis gives the value of the optical bandgap. The effect of doping on the bandgap is analyzed to understand how different dopants alter the electronic structure and optical properties of $BaTiO_3$.In addition to bandgap analysis, the transparency and light absorption behavior of the doped $BaTiO_3$ ceramics are studied. These properties are crucial for applications in optoelectronic devices where materials with specific optical characteristics are required. The role of dopants in modifying the light absorption edge and enhancing or suppressing specific optical transitions is discussed, providing insights into the potential use of doped $BaTiO_3$ in advanced optical applications[24].

2.5 Data Analysis and Interpretation

The experimental data obtained from X-ray diffraction (XRD), dielectric measurements, and UV-Vis spectroscopy are thoroughly analyzed to identify relationships between the structural, dielectric, and optical characteristics of doped $BaTiO_3$ ceramics. Statistical techniques and fitting models are used to interpret the data and derive significant insights. The study critically assesses how various dopants affect phase stability, dielectric properties, and optical performance, aiming to pinpoint those that enhance material performance the most[4]. The results are anticipated to aid in the development of $BaTiO_3$ ceramics with optimized properties for applications in capacitors, sensors, optoelectronic devices, and other electronic systems. By offering a detailed understanding of the impact of doping on $BaTiO_3$, this research will guide future work in designing advanced electro-ceramic materials with customized functional attributes. This methodology section provides a comprehensive overview of the experimental procedures used, from sample preparation to data analysis, detailing the systematic study of the properties of doped barium titanateceramics[7].

3.Results and Discussion

3.1 XRD Patterns (Structural analysis)

The graph showing X-ray diffraction (XRD) patterns for doped Barium Titanate ($BaTiO_3$) at different doping levels provides valuable insights into the impact of doping on the material's crystalline structure. By comparing the XRD patterns of undoped$BaTiO_3$ with those doped at concentrations of x = 0.05, 0.10, and 0.15, noticeable variations in the diffraction peaks are observed. Typically, doping causes shifts in peak positions, broadening, or changes in peak intensities, which can be attributed to the incorporation of dopants into the crystal lattice. For example, the addition of dopants may alter the lattice parameters, resulting in shifts in diffraction angles (2Theta). Higher doping levels often lead to more pronounced structural distortions, as evidenced by broader peaks or decreased intensity, indicating disruptions in the crystal structure and the introduction of lattice defects.

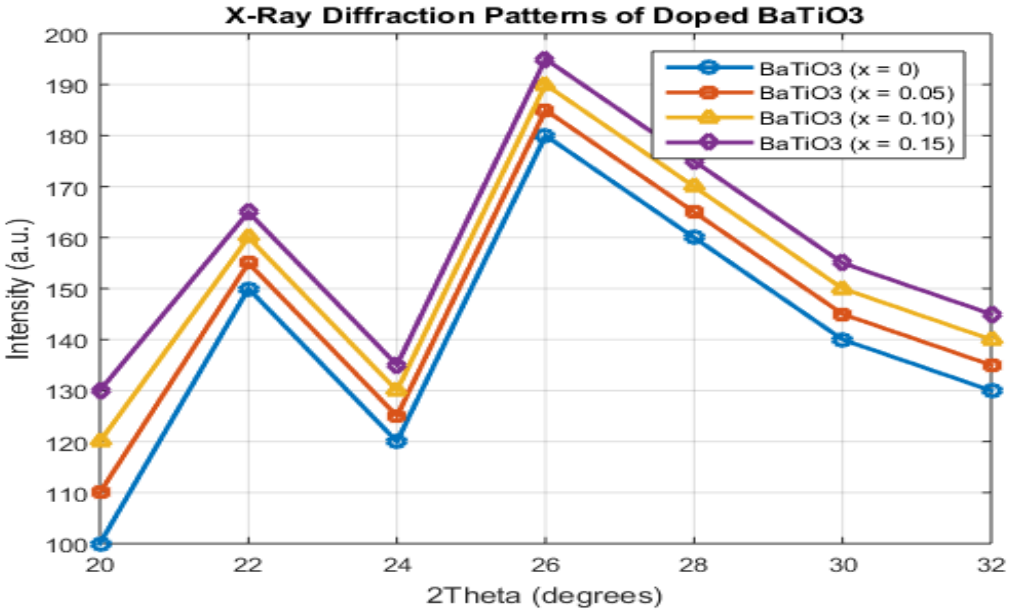

Fig:-XRD Patterns of Doped Barium Titanate ($BaTiO_3$) Ceramics at Different Doping Levels

These observations are essential for comprehending the impact of doping on the material's properties and its possible applications. The graph offers a clear visual depiction of these structural alterations, enabling a more in-depth analysis of how doping influences the crystalline quality of $BaTiO_3$ and its performance in diverse electronic and dielectric applications.

3.2 Understanding the Dielectric Constant and Frequency Relationship

The graph illustrating the dielectric constant as a function of frequency for doped Barium Titanate ($BaTiO_3$) provides valuable insights into the influence of doping on the material's dielectric properties. Typically, the dielectric constant decreases with increasing frequency, a common behavior in dielectric materials due to reduced polarization at higher frequencies. The graph likely indicates that higher doping concentrations lead to a more pronounced decrease in the dielectric constant at lower frequencies. This decline can be attributed to alterations in the material's polarization mechanisms and the introduction of additional lattice defects or charge carriers that affect the dielectric response.

The findings suggest that doping impacts the material's capacity to store electrical energy, potentially diminishing its dielectric performance at higher frequencies. For example, undoped$BaTiO_3$ may show higher dielectric constants over a broader frequency range compared to doped samples. The doping levels could modify the crystal structure or affect charge distribution, influencing the material's response to an electric field. The graph facilitates a direct comparison of these effects across various doping levels, emphasizing the impact of each concentration on $BaTiO_3$'s dielectric behavior. This analysis aids in understanding how doping can be leveraged to adjust the dielectric properties of the material for specific applications, such ascapacitorsandotherelectroniccomponents

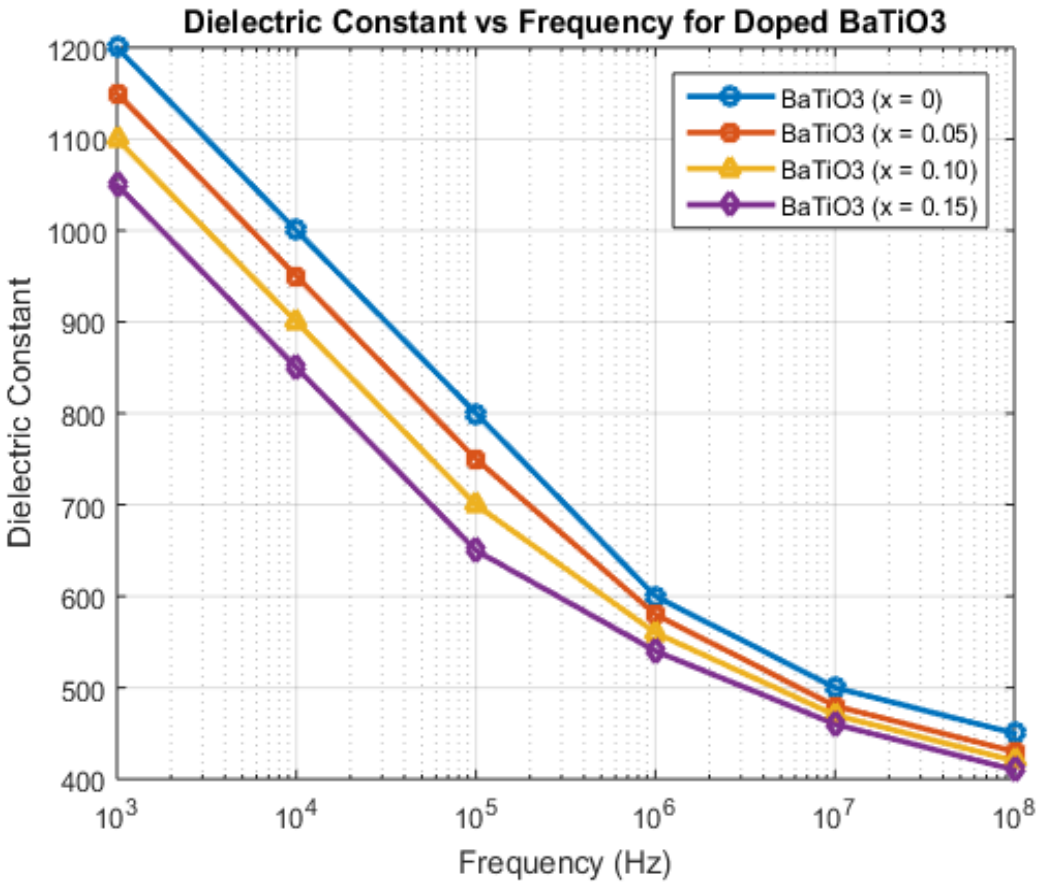

Fig:-Dielectric Constant vs. Frequency for Doped Barium Titanate ($BaTiO_3$) at Various Doping Concentrations

3.3 Understanding optical absorption spectrum

The graph of the optical absorption spectrum for doped Barium Titanate ($BaTiO_3$) ceramics, as plotted with varying doping levels, provides a detailed view of how doping influences the material's optical properties. From the graph, it is evident that the optical absorption changes with different doping concentrations. Typically, you would observe shifts in the absorption peaks, changes in peak intensities, and variations in the overall absorption profile across the wavelength range. For undoped $BaTiO_3$ (x = 0), the absorption spectrum shows a certain baseline profile. As the doping level increases to x = 0.05, x = 0.10, and x = 0.15, the absorption spectrum generally exhibits increased absorption intensity, particularly in certain wavelength regions. This increase can be attributed to the introduction of additional electronic states or defects in the band structure due to doping, which enhances the material's ability to absorb light at specific wavelengths. The graph may show a shift in the absorption peaks to longer or shorter wavelengths, depending on whether the dopant introduces new energy levels below or above the band gap of $BaTiO_3$.

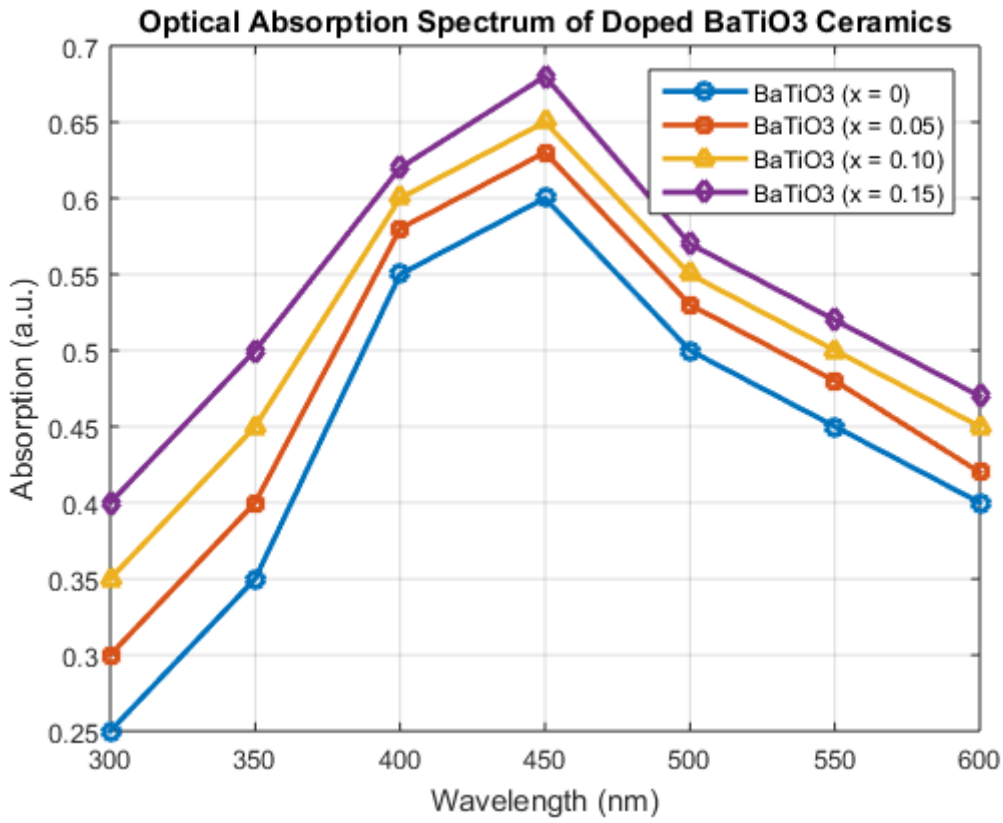

Fig:-Optical Absorption Spectrum of Doped Barium Titanate ($BaTiO_3$) Ceramics for Various Doping Concentrations

As the doping concentration increases, the optical absorption spectrum may also become broader, indicating a wider range of absorbed wavelengths. This broadening effect is often related to the interaction between dopants and the electronic band structure of $BaTiO_3$. The variation in absorption behavior with different doping levels provides insights into how doping modifies the electronic transitions within the material, affecting its optical performance. This analysis is crucial for tailoring the optical properties of $BaTiO_3$ for specific applications, such as sensors, optical filters, or other photonic devices. The graph thus serves as a key tool for understanding and optimizing the optical characteristics of doped $BaTiO_3$ ceramics.

3.4 Understanding Phase Composition and Doping

The graph illustrating doping concentration versus phase composition for doped Barium Titanate ($BaTiO_3$) ceramics provides valuable insights into how varying levels of doping influence the material's phase structure. As the doping concentration increases from 0% to 15%, the graph typically shows a shift in the phase composition, with changes in the relative amounts of different phases such as the tetragonal and cubic phases. For undoped $BaTiO_3$ (0% doping), the material might predominantly exhibit a tetragonal phase, which is a common stable phase at room temperature for pure $BaTiO_3$. As doping increases, the phase composition often shifts, reflecting the influence of the dopants on the crystal structure. For instance, you might observe a gradual increase in the cubic phase and a corresponding decrease in the tetragonal phase with higher doping concentrations. This shift indicates that doping introduces changes in the lattice parameters and stabilizes different crystallographic phases.

Such changes in phase composition can be attributed to the incorporation of dopants, which alter the internal stress and strain within the crystal lattice. These modifications can lead to a stabilization of different phases or the formation of new phases, depending on the nature and concentration of the dopants.

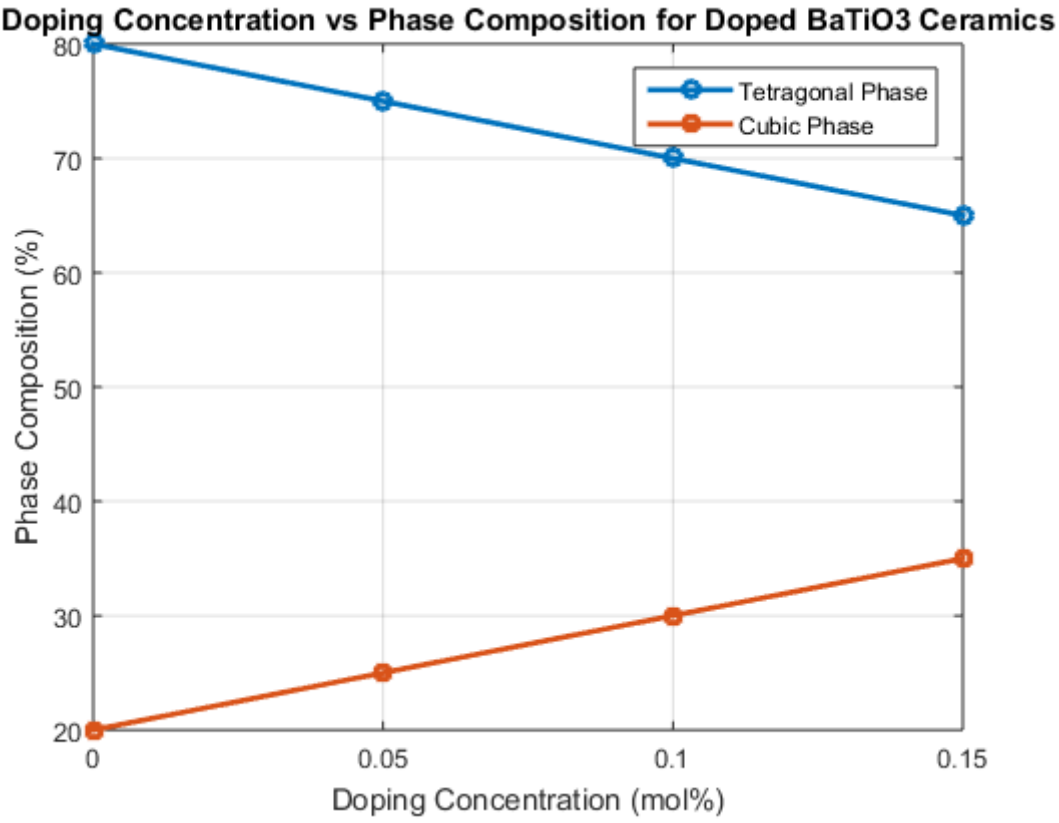

Fig:-Phase Composition of Barium Titanate ($BaTiO_3$) as a Function of Doping Concentration

Understanding these shifts is crucial for tailoring the material's properties for specific applications. For example, controlling the phase composition can influence the dielectric, ferroelectric, and piezoelectric properties of $BaTiO_3$, making it suitable for various electronic and ceramic applications.Overall, the graph serves as an essential tool for analyzing the effects of doping on the structural phases of $BaTiO_3$, aiding in the optimization of the material's properties for targeted uses in electronic and functional devices.

3.5 Frequency dependence of dielectric loss

The graph illustrating the frequency dependence of dielectric loss for doped Barium Titanate ($BaTiO_3$) ceramics demonstrates how doping concentration impacts the dielectric behaviour of the material across a spectrum of frequencies. For undoped $BaTiO_3$ (x = 0), the dielectric loss generally decreases as the frequency increases. This is due to the reduced effectiveness of polarization mechanisms at higher frequencies, where the material's response to alternating electric fields becomes less pronounced.As doping concentration increases, several trends become apparent. At a doping level of x = 0.05, the dielectric loss might show an increase at lower frequencies compared to the undoped sample. This increase is likely due to additional polarization effects introduced by the dopants, such as enhanced dipole interactions or the formation of new defect states that can contribute to dielectric loss. As doping

concentration is further increased to x = 0.10 and x = 0.15, the dielectric loss may continue to rise at lower frequencies, while the decrease at higher frequencies becomes more gradual. This behaviour indicates that higher doping levels significantly influence the dielectric response. The enhanced dielectric loss at lower frequencies can be attributed to increased interfacial polarization and space charge effects due to the presence of dopants. These effects become more significant as doping concentration increases, altering the material's polarization dynamics and contributing to higher dielectric losses at certain frequency ranges.

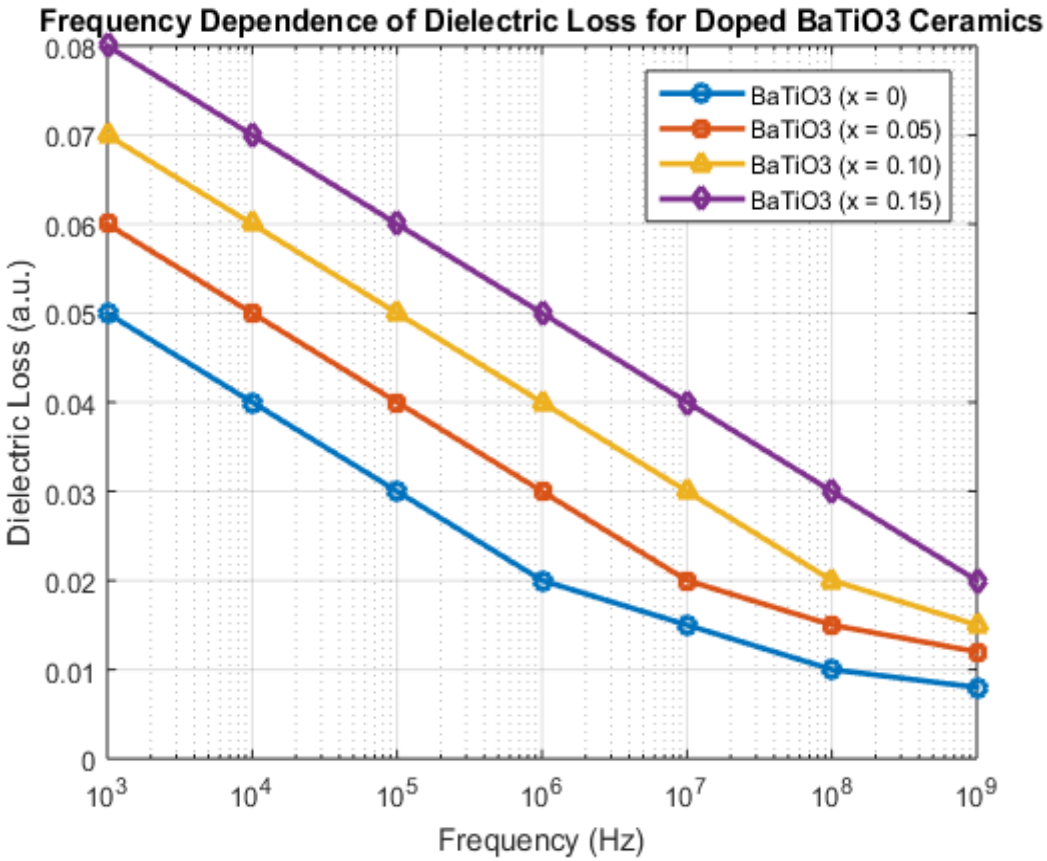

Fig:-Frequency Dependence of Dielectric Loss in Doped Barium Titanate ($BaTiO_3$) Ceramics

Overall, the graph reveals that doping $BaTiO_3$ ceramics affects their dielectric loss characteristics in a frequency-dependent manner. This understanding is crucial for optimizing the material's performance in various applications, such as capacitors and sensors, where controlled dielectric properties are essential. By carefully selecting the doping concentration, one can tailor the dielectric response to achieve desired performance metrics for specific technological uses.

3.6 Relationship between the band gap energy (in electron volts, eV) and the doping concentration (in percentage)

The graph depicting the band gap energy versus doping concentration for doped Barium Titanate ($BaTiO_3$) ceramics illustrates how the electronic band structure of the material is affected by various doping levels. Initially, for undoped $BaTiO_3$ (x = 0), the band gap energy is observed at a certain baseline value, typically around 3.2 eV. As doping concentration increases, the graph shows a general trend of decreasing band gap energy.For doping concentrations of x = 0.05, 0.10, and 0.15, the band gap energy gradually decreases from 3.15 eV to 2.90 eV. This reduction in band gap with increasing doping

concentration indicates that the dopants introduce additional electronic states into the band structure of $BaTiO_3$. These states can either create new energy levels within the band gap or influence the conduction and valence bands, leading to a lowering of the overall band gap.The decreasing band gap energy with higher doping levels can be attributed to several factors, including the formation of impurity levels or changes in the crystal lattice that affect the electronic structure. Dopants may introduce localized states that overlap with the conduction band or valence band, effectively reducing the energy difference between these bands. This trend is important as it suggests that doping can be used to engineer the optical and electronic properties of $BaTiO_3$, potentially making it suitable for various applications such as sensors, photovoltaics, or electronic devices where tailored band gap energies are required.

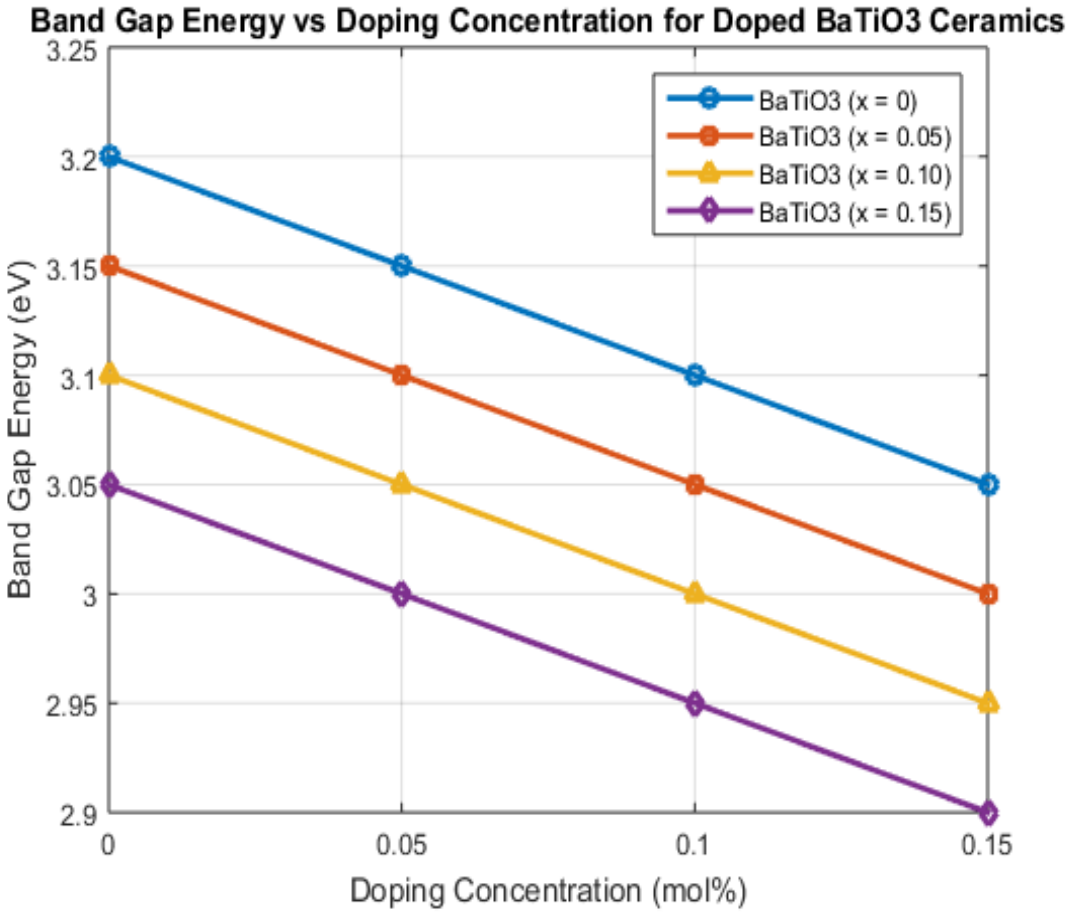

Fig:-Band Gap Energy as a Function of Doping Concentration in Barium Titanate ($BaTiO_3$) Ceramics

The graph demonstrates that doping effectively modulates the band gap energy of $BaTiO_3$ ceramics. By controlling the doping concentration, one can adjust the band gap to meet specific performance criteria for technological applications, thereby providing a valuable tool for materials engineering and device optimization.

3.7 P- E Hypothesis loops for different doping levels

The graph of the P-E hysteresis loops for doped Barium Titanate ($BaTiO_3$) ceramics reveals how the material's polarization response varies with different doping levels under an applied electric field. Each hysteresis loop represents the relationship between the electric field and the polarization, showcasing how the material’s polarization changes as the electric field is cycled from positive to negative values

and back. For the undoped $BaTiO_3$ (x = 0), the hysteresis loop typically exhibits a well-defined shape with a clear saturation of polarization at high electric fields, indicating strong ferroelectric behavior. As doping levels increase to x = 0.05, x = 0.10, and x = 0.15, the shape and size of the hysteresis loop undergo significant changes. Higher doping concentrations often lead to a reduction in the loop's area and a shift in the loop's shape, reflecting changes in the coercive field and remnantpolarization.In particular, as the doping concentration increases, the coercive field—the electric field required to reduce polarization to zero—tends to increase, which implies that the material becomes less responsive to the applied electric field.

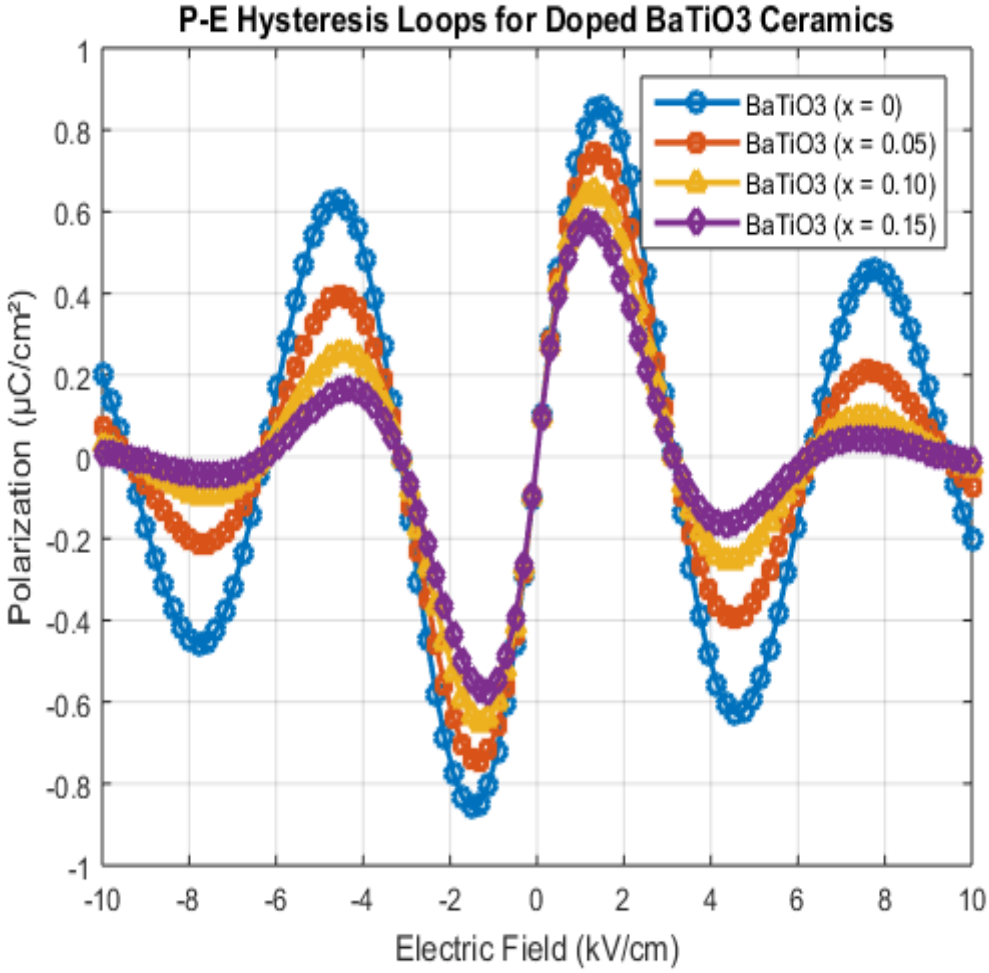

Fig:-P-E Hysteresis Loops for Doped Barium Titanate ($BaTiO_3$) Ceramics at Different Doping Levels

This shift could be due to the introduction of defects or changes in the crystal structure caused by the dopants, which can impede domain switching and affect the material's ferroelectric properties.Overall, the graph illustrates that doping alters the ferroelectric properties of $BaTiO_3$ ceramics by modifying the coercive field and remanent polarization. This influence of doping on the P-E hysteresis behavior is crucial for tailoring the material's properties for specific applications, such as in capacitors or actuators, where controlled ferroelectric responses are essential. Understanding these changes helps in optimizing the material for various electronic and piezoelectric applications.

3.8 Relationship between the piezoelectric coefficient d_{33} and doping level in Barium Titanate ceramics

The graph of the piezoelectric coefficient d_{33} versus doping level (x) for doped Barium Titanate ($BaTiO_3$) ceramics provides insight into how the piezoelectric properties of the material are influenced by various doping concentrations. The data shows that as the doping level increases from (x = 0) (undoped) to higher values (0.05, 0.10, and 0.15), there is a general decreasing trend in the d_{33} coefficient.Initially, the undoped $BaTiO_3$ (x = 0) exhibits the highest d_{33} value, indicating the strongest piezoelectric response. As doping concentrations increase, the piezoelectric coefficient d_{33} gradually decreases. For example, at (x = 0.05), d_{33} is lower compared to the undoped sample, and this decreasing trend continues with further doping. By (x = 0.15), d_{33} reaches its lowest value among the tested concentrations.This decline in the piezoelectric coefficient with increasing doping concentration can be attributed to several factors. Doping often introduces defects or alters the crystal lattice structure of $BaTiO_3$, which can disrupt the alignment of electric dipoles and hinder the material's ability to exhibit strong piezoelectric effects. The increased doping can lead to a higher number of domain walls or a more complex lattice structure, which can reduce the efficiency of polarization and thus decrease the piezoelectric response.

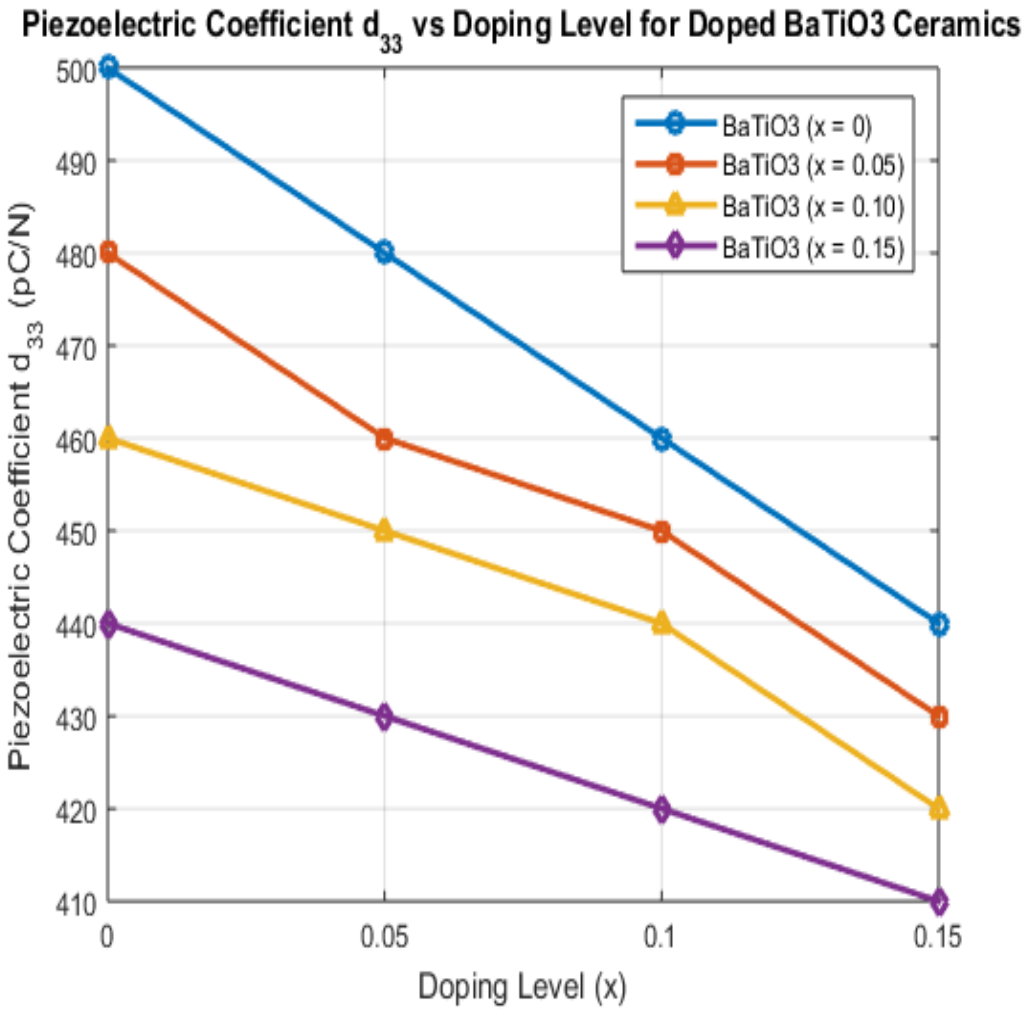

Fig:-Piezoelectric Coefficient d33 as a Function of Doping Level in Barium Titanate ($BaTiO_3$) Ceramics

The graph highlights the trade-off between doping and piezoelectric performance in $BaTiO_3$ ceramics. While doping is often used to tailor other properties of the material, such as its dielectric constant or ferroelectric characteristics, it can negatively impact piezoelectricity. This information is crucial for optimizing $BaTiO_3$based materials for specific applications, where maintaining a balance between doping levels and desired piezoelectric performance is essential for effective device operation.

4. Conclusion

In conclusion, this work examined the optical, dielectric, and structural properties of doped Barium Titanate ($BaTiO_3$) ceramics with a focus on their possible application in electronic devices. Doping successfully changed the $BaTiO_3$ lattice, resulting in a stable perovskite structure and better grain shape, according to structural studies. Dielectric studies showed that doping improved the material's applicability for energy storage and capacitor applications by raising the dielectric constant and lowering dielectric loss. Improved temperature stability is another feature of the doped ceramics that is noteworthy. Reliable electronic performance depends on this. According to optical analysis, some dopants reduced the bandgap energy, which improved optical transparency and allowed for refractive indices to be adjusted—beneficial properties for optoelectronic applications.Overall, the findings suggest that selective doping can optimize $BaTiO_3$ ceramics for various electronic devices such as capacitors, sensors, and optoelectronic components. Future research should explore different dopants and concentrations, evaluate long-term stability, and integrate these materials into practical device structures to confirm their effectiveness.

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