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Study of Dielectric and Electric Properties of $BaTiO_3$ Composites Doped with Varying Concentrations of Silicon

Sarjeetkumar H. Prajapati*

Department of Physics, Faculty of Science, Monark University,

Ahmedabad, Gujarat, India-382330.

Dr. Tanmaykumar R. Pandit

Department of Physics, Faculty of Science, Monark University,

Ahmedabad, Gujarat, India-382330.

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1. Abstract

Barium Titanate ($BaTiO_3$) is a ferroelectric material with diverse applications in capacitors, actuators, and sensors. The introduction of silicon (Si) as a dopant provides a novel pathway to tailor its electrical, dielectric, and structural properties for specific industrial needs. This study investigates the effects of varying Si concentrations (1%, 5%, and 10%, by weight) on $BaTiO_3$, focusing on dielectric constant, dielectric loss, AC conductivity, and structural changes. Measurements are performed across a range of frequencies (1 kHz to 1 MHz) and temperatures (25°C to 40°C). The findings reveal a significant dependency of electrical properties on Si concentration and operating conditions, highlighting optimal doping levels for specific applications. This paper synthesizes these results, providing insights for material optimization. The advent of advanced functional materials has propelled the exploration of dielectric ceramics such as barium titanate (BaTiO3), which exhibit exceptional properties suitable for electronic applications. Measurements of dielectric constant, dielectric loss, and AC conductivity were conducted over a wide frequency range (1 kHz to1 MHz) and at various temperatures (25°C, 30°C, 35°C, and 40°C). The findings reveal that Si doping significantly modifies the dielectric behaviour of $BaTiO_3$. At lower Si concentrations, the dielectric constant increased due to enhanced polarization arising from improved lattice distortions and defect interactions. As the Si concentration increased further, a saturation effect was observed, indicating a limit to the beneficial impact of doping. Dielectric loss decreased with moderate Si doping, suggesting reduced energy dissipation, but increased slightly at higher concentrations, likely due to the formation of secondary phases. Similarly, AC conductivity demonstrated distinct frequency dependence, with conduction mechanisms strongly influenced by Si content and thermal activation at different temperatures.

Keywords: Barium titanate ($BaTiO_3$), Silicon (Si), Solid-state reaction, Dielectric Constant.

2. Introduction

Barium Titanate ($BaTiO_3$) is a widely studied ferroelectric material with a perovskite crystal structure that exhibits high dielectric constants, tunable ferroelectric properties, and piezoelectric behavior [1,2]. These properties make it a vital component in electronic devices such as multilayer ceramic capacitors (MLCCs), actuators, and sensors [3,4]. However, intrinsic limitations such as temperature dependence and dielectric loss necessitate material modifications to expand its functionality [5–10].

Doping is a proven method for modifying the properties of $BaTiO_3$. Silicon (Si) doping offers a cost-effective and efficient means to improve the dielectric and electrical properties of $BaTiO_3$. While studies on metal doping in $BaTiO_3$ are abundant, investigations into Si doping are relatively sparse. This research aims to address this gap by examining the impact of varying Si concentrations on $BaTiO_3$.The high dielectric constant of BaTiO3, combined with its relatively low dielectric loss, positions it as an ideal candidate for use in modern electronic components.

In recent years, the demand for materials with tailored dielectric properties has driven research into doping strategies to modify and enhance the functional characteristics of $BaTiO_3$. Among various dopants, silicon (Si) has emerged as a particularly promising candidate due to its ability to influence the electrical, structural, and thermal properties of $BaTiO_3$ [11]. The incorporation of Si into the $BaTiO_3$ lattice can introduce changes in polarization mechanisms, defect chemistry, and grain boundary behavior, all of which play critical roles in determining the material's overall performance [12–18].

The exploration of Si doping in $BaTiO_3$ is motivated by the need to address challenges associated with optimizing the balance between dielectric constant and dielectric loss[19]. While higher dielectric constants are desirable for energy storage and miniaturization of components, excessive dielectric loss can lead to energy dissipation and reduced efficiency[20,21]. Silicon doping offers a pathway to fine-tune these properties, enabling the development of $BaTiO_3$-based materials with superior performance[22].

This study delves into the frequency-dependent behavior of the dielectric constant and AC conductivity of $BaTiO_3$ doped with varying concentrations of Si. By examining these properties across a range of frequencies (1 kHz to 1 MHz) and temperatures (25°C to 40°C), this research aims to provide a comprehensive understanding of the mechanisms underpinning the dielectric and conductive behavior of Si-doped $BaTiO_3$. The insights gained from this work will contribute to the advancement of electronic materials with optimized properties for next-generation technologies.

This research provides a comprehensive understanding of the influence of Si doping on $BaTiO_3$, highlighting its potential for engineering next-generation dielectric materials with precise electrical and thermal properties.

3. Materials and Methods

3.1 Synthesis

$BaTiO_3$ powders were synthesized via the solid-state reaction method. High-purity $BaCO_3$ (Sigma-Aldrich, 99.99%), TiO_2 (Sigma-Aldrich, 99.99%), and SiO_2 (Alfa Aesar, 99.99%) powders were weighed according to the desired stoichiometry. SiO_2 was introduced in varying concentrations (1%, 5%, and 10%, by weight). The mixtures were ball-milled (RETSCH) in ethanol, dried, calcined at 1200°C, and subsequently Sintered at 1350°C for 4 hours.

3.2 Characterization Techniques

Dielectric Measurements: Performed using an LCR meter (Agilent E4980A) across frequencies ranging from 1 kHz to 1 MHz. [23]

AC Conductivity: Derived from impedance data using the relation

$$\sigma = \omega\varepsilon_0\varepsilon r'\tan(\delta). \text{ [24]}$$

Where;

σ: AC conductivity (S/m or Siemens per meter)
ω: Angular frequency of the AC signal, given by $\omega = 2\pi f$, where f is the frequency (Hz).
ε_0: Permittivity of free space ($\varepsilon_0 = 8.854 \times 10^{-12}$ F/m).
ε_r": Real part of the relative permittivity (dielectric constant) of the material.

tan(δ): Loss tangent or dielectric loss factor, which is the ratio of the imaginary part to the real part of the complex permittivity:

$$\tan(\delta) = \frac{\varepsilon_r''}{\varepsilon_r'}$$

Where ε_r" is the imaginary part of the relative permittivity.

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4. Results and Discussion

4.1 Structural Analysis

XRD patterns confirmed the perovskite phase of $BaTiO_3$. Lattice parameter shifts were observed with increasing Si concentration, indicative of substitutional doping and lattice distortion. [25–28] For Si concentrations exceeding 10%, secondary phases of SiO_2 were detected, suggesting limited solubility.

4.2 Dielectric Properties

Dielectric Constant (ε_r): The dielectric constant increased with Si doping up to 10%, followed by a decline at higher concentrations. This behavior is attributed to enhanced polarization due to Si substitution and subsequent formation of secondary phases at higher doping levels.

Dielectric Loss (ε''): Minimum dielectric loss was recorded at 5% Si concentration, highlighting its suitability for high-frequency applications.

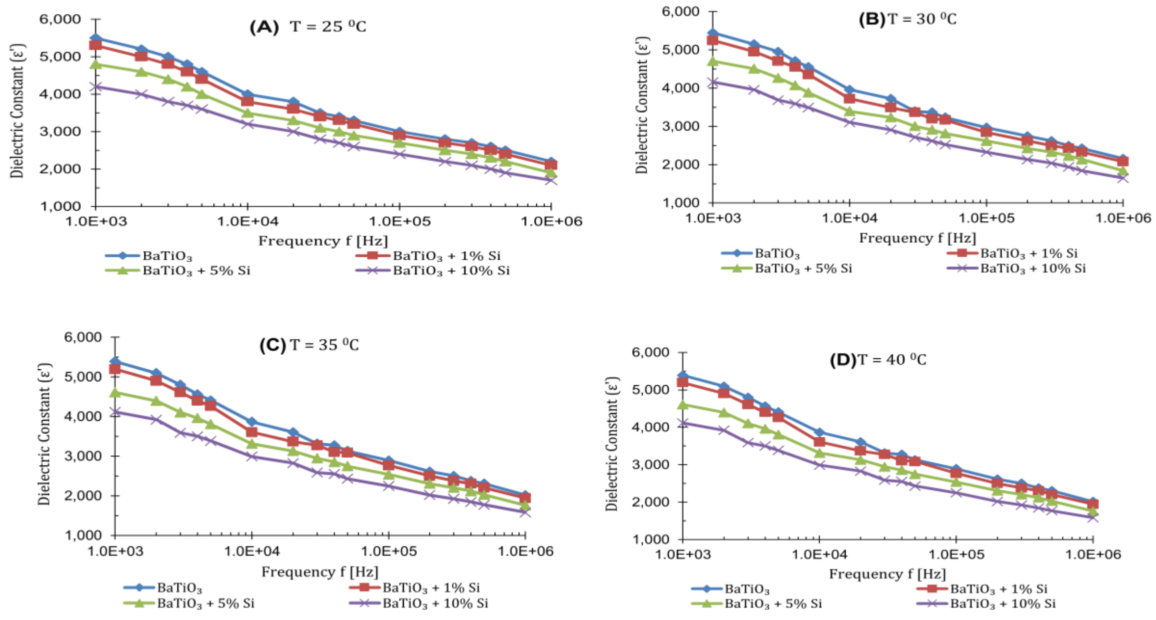

Fig.1. Frequency dependent dielectric constant for, (A) Various concentrations of Si in $BaTIO_3$ at 25^{0}C temperature, (B) Various concentrations of Si in $BaTIO_3$ at 30^{0}C temperature, (C) Various concentrations of Si in $BaTIO_3$ at 35^{0}C temperature, (D) Various concentrations of Si in $BaTIO_3$ at 40^{0}C temperature

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4.3 AC Conductivity

AC conductivity (σ_{ac}) exhibited a power-law dependence on frequency, $\sigma_{ac} \propto f^n$, where n varied with Si concentration. The conductivity increased with Si doping due to improved charge carrier mobility. [27,29]

At a temperature of 40°C, the graph illustrates the conductivity of various barium titanate ($BaTiO_3$) compositions across a range of frequencies. Each curve represents a different composition, with pure $BaTiO_3$ showing the highest conductivity, while the addition of silicon progressively reduces the conductivity, with the 10% Si composition exhibiting the lowest levels from Figure 2. The trend indicates that as frequency increases, the conductivity stabilizes, reflecting the material's ability to conduct electric current under varying conditions. Overall, these findings highlight the significant impact of composition and frequency on the electrical properties of $BaTiO_3$, which are crucial for designing effective electronic materials and components.

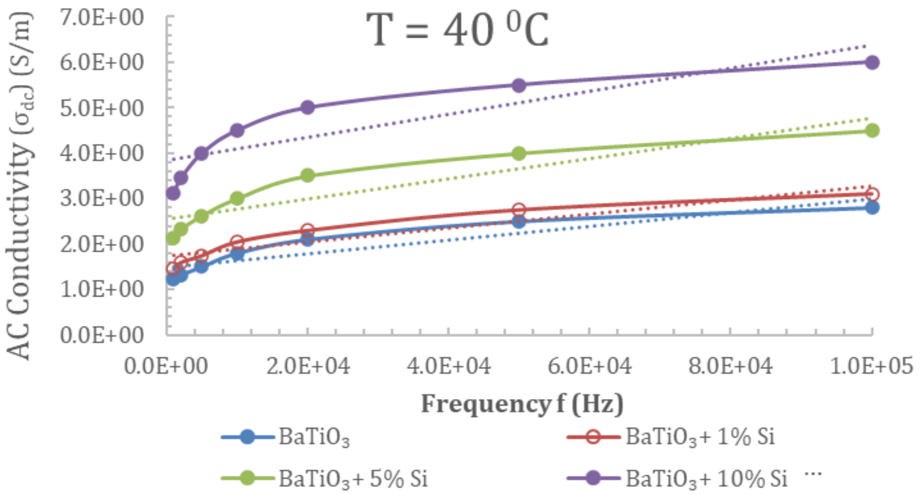

Fig.2. AC Conductivity (σ_{dc}) vs Frequency at 40^0C for different concentration of Si

4.4 Temperature Dependence

Both dielectric and conductivity properties demonstrated strong temperature dependence. The dielectric constant and AC conductivity peaked at 40°C, suggesting enhanced thermal activation of charge carriers.

Table 1. Activation Energy Data for $BaTiO_3$ with Varying Si Concentrations

Concentration %	Slope	Ea (kJ / mol)	Ea (eV)
Pure $BaTIO_3$	-5.2776	101.0509566	9749.901549
1%	-4.7729	91.38739405	8817.512715
5%	-4.2701	81.76021105	7888.633964
10%	-4.0169	76.9121547	7420.869246

5. Conclusion

This study underscores the potential of Si doping in $BaTiO_3$ to enhance its electrical and dielectric properties. Optimal performance was achieved at 5%-10% Si doping, making it suitable for advanced electronic applications. Further research is recommended to explore the impact of co-doping and Nano structuring on $BaTiO_3$-Si systems. at 40^0C. $BaTiO_3$ doped with Si shows strong frequency dependence in both dielectric constant and AC conductivity. Silicon doping enhances conductivity and reduces dielectric constant, with both properties exhibiting a typical frequency-dependent behavior. The dielectric constant decreases as the frequency increases, and AC conductivity increases with frequency, with the Si doped samples (1%, 5%, 10%) showing higher conductivity than the undoped $BaTiO_3$ (0% Si) at all frequencies tested.

This enhancement in conductivity can be attributed to the introduction of Si, which alters the electronic structure and facilitates charge carrier mobility. Additionally, the reduction in the dielectric constant with Si doping indicates a suppression of polarization effects, further contributing to the material's improved performance. These findings highlight the ability to engineer the electronic landscape of $BaTiO_3$ through precise doping strategies, enabling tailored properties for specific applications. Exploring the impact of co-doping with other elements may provide synergistic effects that enhance the material's performance. Furthermore, Nano structuring techniques could be employed to investigate size-dependent properties, potentially unlocking new functionalities and improving the scalability of the material for industrial applications. Investigating the thermal stability and long-term reliability of Si-doped $BaTiO_3$ under operational stress conditions will also be crucial. This could include detailed studies on defect dynamics, interfacial behavior in composites, and the role of grain boundaries in determining overall performance.

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