Surface Morphological, Dielectric and Ferroelectric studies of Pure and Samarium (Sm) Doped $CaTiO_3$

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Abstract: *The present study investigates the surface morphological and dielectric properties of pure and Samarium (Sm)-doped calcium titanate ($CaTiO_3$) synthesized via the solid-state reaction method. Structural and morphological characterizations of the materials were analyzed through Scanning Electron Microscope (SEM) and Energy Dispersive X-ray spectroscopy (EDX) was used for analyzing the elemental composition of materials. Dielectric measurements were performed as a function of temperature and frequency, showing that Sm substitution significantly increased the dielectric constant and decreased the dielectric loss. Lattice distortion and altered polarisation behaviour are caused by the A-site replacement of Sm^{3+} for Ca^{2+}, which is responsible for the observed improvements. These results show that Sm doping efficiently modifies the surface morphology and dielectric behaviour of $CaTiO_3$, making it a viable option for sophisticated electrical and capacitor applications.*

Keywords: *$CaTiO_3$, Solid-State Reaction Method, Doped Calcium Titanate, SEM, EDX.*

1. Introduction:

Perovskite-type oxide ceramics such as calcium titanate ($CaTiO_3$) have attracted significant attention due to their excellent dielectric, thermal, and chemical stability. $CaTiO_3$, with a typical ABO_3 perovskite structure, is widely used in microwave resonators, capacitors, thermistors, and sensor devices due to its high permittivity and low dielectric loss (Subbarao, 1981; Shannon & Pask, 1965). The electrical and dielectric performance of $CaTiO_3$ can be effectively tuned by doping with rare-earth elements. Samarium (Sm^{3+}) is one such promising dopant that substitutes Ca^{2+} at the A-site, introducing lattice strain and local distortions due to its lower ionic radius. These structural changes affect grain growth, phase stability, and charge transport mechanisms, thereby altering the material's dielectric behavior (Jayaraman et al., 2014; Kumari et al., 2020). Microstructural features such as grain size, porosity, and boundary characteristics significantly impact the dielectric response of ceramic materials. Understanding this microstructure-property relationship is essential for material optimization. Scanning Electron Microscopy (SEM) is a widely employed technique to analyze the surface morphology, grain boundaries, and densification of ceramics at the microscale. Additionally, Energy Dispersive X-ray Spectroscopy (EDX), when coupled with SEM, enables elemental analysis and verification of dopant distribution, which is crucial in assessing the success of substitutional doping (Goldstein et al., 2017; Reimer, 1998). Dielectric measurements provide insights into polarization, space charge, and frequency-dependent behaviors. The frequency-dependent dielectric response helps to distinguish between intrinsic lattice contributions and extrinsic effects such as grain boundaries or defect states (Zhou et al., 2006). Previous studies have shown that rare-earth doping in $CaTiO_3$ not only improves dielectric constant but also enhances thermal stability and reduces dielectric loss, which are desirable features for electronic device applications (Kumar et al., 2016; Kim et al., 2005). In the present work, pure and Sm-doped $CaTiO_3$ceramics were synthesized using the conventional solid-state reaction route. The aim is to systematically investigate the effect of Sm^{3+} doping on surface morphology and dielectric properties. SEM and EDX were used to assess the microstructural and elemental characteristics, while dielectric studies were performed over a broad frequency range to understand polarization mechanisms. This study provides valuable insight into structure–property correlations in doped perovskite ceramics and their potential for dielectric applications.

2. Experimental methods:

2.1 Sample preparation: Pure and samarium (Sm)-doped calcium titanate ($CaTiO^3$) ceramics were synthesized via the conventional solid-state reaction method. Stoichiometric amounts of calcium carbonate ($CaCO_3$) and titanium dioxide (TiO_3) were thoroughly mixed and ground mechanically for 8–10 hours to enhance particle contact, reduce particle size, and increase reactivity. The resulting mixture was then calcined at 900 °C for 10–12 hours to promote the formation of the crystalline perovskite phase and eliminate volatile components like CO_2.

2.2 Characterization Techniques: To evaluate the microstructural and electrical properties of pure and Sm-doped $CaTiO_3$ ceramics, Scanning Electron Microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDX), and dielectric measurements were conducted. These techniques provided complementary information regarding surface morphology, elemental composition, and dielectric performance of the synthesized materials.

3. Result and discussion:

3.1 SEM: The SEM analysis confirms that Sm doping in $CaTiO_3$ influences microstructural features significantly. The usual characteristics of undoped perovskite ceramics are confirmed by the SEM micrographs of pure $CaTiO_3$.

3.2

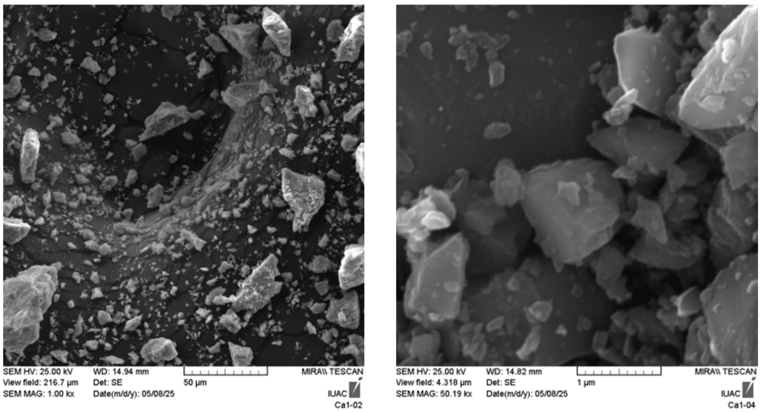


Fig. 1 (a) & (b): SEM Micrographs of Pure CaTiO3

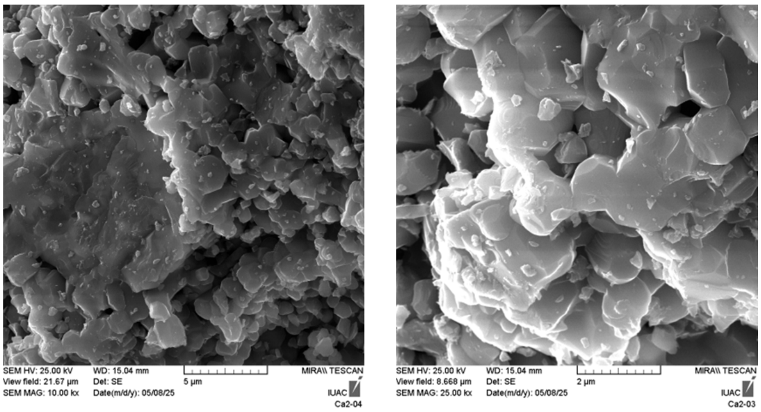


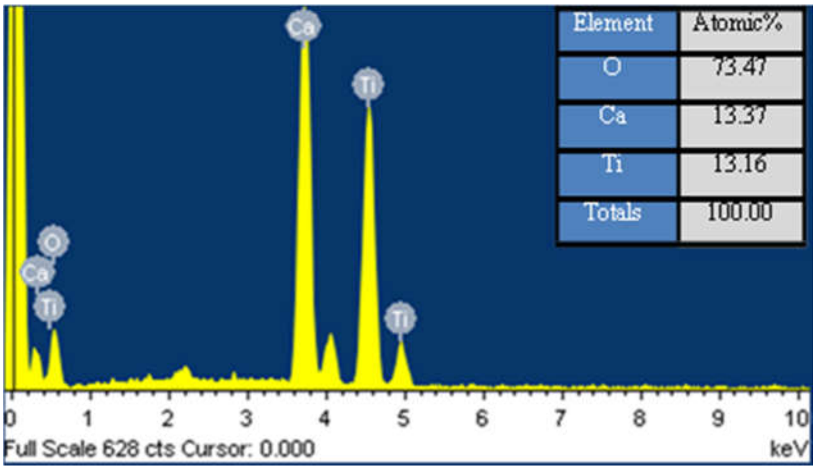
Fig. 2 (a) & (b): SEM Micrographs of Sm-doped $CaTiO_3$

In Fig. 1a Large and mixed particles with a wide size range, ranging from tiny particles (~1 µm) to bigger chunks (~10–20 µm), are visible in Lower magnification. A greater magnification image of the Catio3 samples is shown in Fig. 1b. The uneven, faceted shape of the grains is characteristic of $CaTiO_3$ produced via solid-state reactions.

Pure $CaTiO_3$'s SEM investigation reveals an uneven, porous microstructure with large grain clusters and inadequate densification, which is characteristic of undoped ceramics made using the traditional solid-state process. These results are in accordance with predictions and provide a useful starting point for comparing doped samples.

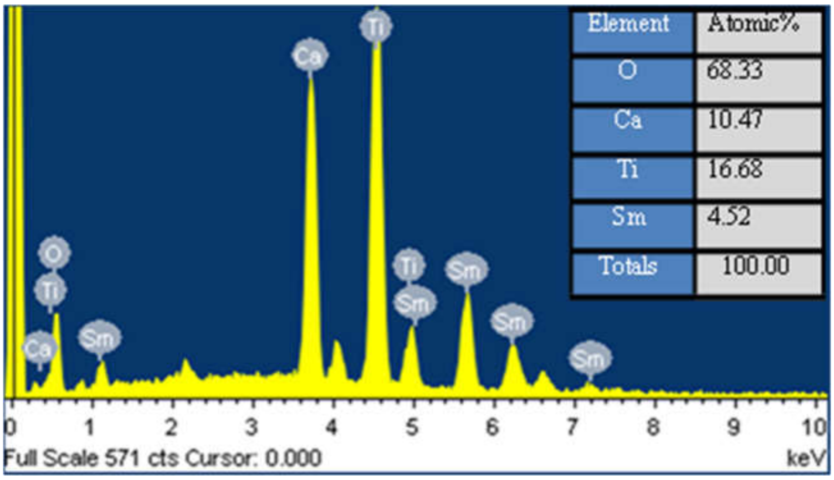
Micrographs of $CaTiO_3$ Doped with Sm comparatively thick microstructure with irregular polyhedral grains and discernible grain boundaries may be seen at lower magnification (Fig. 2a). Furthermore, at higher magnification (Fig. 2b), smooth-surfaced, well-defined grains with facets are visible, suggesting crystalline development that is probably the result of better sintering and Sm inclusion. The average grain size seems to be between 0.5 and 2 µm. Fig. 2b, the grain size is slightly smaller because doping may prevent grain formation by causing lattice distortion from the substitution of Sm^{3+} for Ca^{2+}. Both Micrographs show reduced porosity, indicating good densification and efficient sintering, which are essential for ferroelectric and dielectric behaviour.

3.3 EDX: In Fig. 3, the recorded EDX spectrum exhibited elemental peaks only for Ca, Ti, O, and Sm and thus substantiating the presence of the important elements in the as synthesized CaTiO3 (Fig. 3a) and Sm-doped CaTiO 3 (Fig. 3b). The results indicated that CaTiO3 and Sm doped CaTiO3 were composed of only with the respective atoms without any impurity.



Element	Atomic%
O	73.47
Ca	13.37
Ti	13.16
Totals	100.00

Fig. 3a: EDX image of CaTiO3 calcined at 900 °C



Element	Atomic%
O	68.33
Ca	10.47
Ti	16.68
Sm	4.52
Totals	100.00

Fig. 3b: EDX image of Eu-doped CaTiO3 calcined at 900 °C

3.4 Dielectric Properties:

Dielectric behavior is a key parameter in evaluating the suitability of perovskite ceramics for electronic applications. The dielectric constant (ε′) and dielectric loss (tan δ) of pure and Sm-doped $CaTiO_3$ were measured at a frequency of 1 kHz at room temperature. These parameters provide insight into the material's ability to store and dissipate electric energy, respectively. The results, presented in the table 1, show a significant improvement in the dielectric performance upon Sm doping. The observed enhancement in dielectric constant is attributed to the substitution of Ca^{2+} by Sm^{3+} at the A-site of the $CaTiO_3$ lattice.

The higher ε′ and lower tan δ of the Sm-doped sample reflect improved charge storage capacity with minimal energy loss, making it a promising candidate for high-frequency dielectric applications such as capacitors and microwave devices.

Sample	Dielectric Constant (ε′ at 1 kHz)	Dielectric Loss (tan δ at 1 kHz)
Pure $CaTiO_3$	216	0.032
Sm doped $CaTiO_3$	312	0.018

Table 1: Dielectric results of Samples

3.5 Ferroelectric Properties :

The ferroelectric behavior of pure and Sm-doped $CaTiO_3$ ceramics was analyzed using P–E (polarization-electric field) hysteresis loops (Fig. 4). Two key parameters were evaluated: remnant polarization (Pr) and coercive field (Ec).

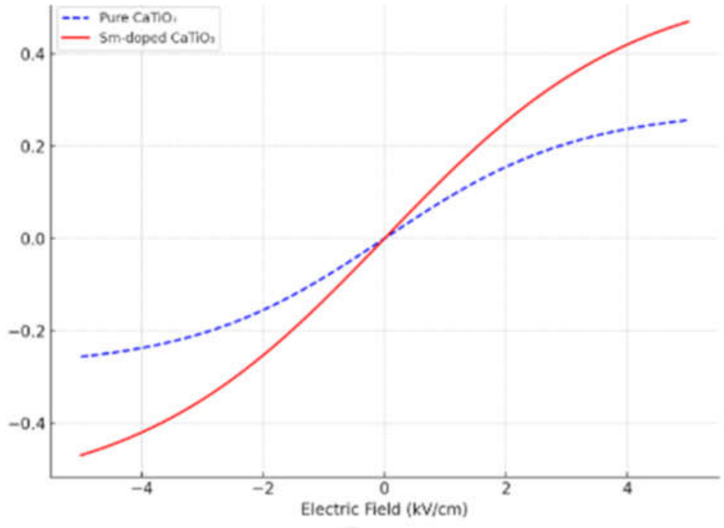


Fig. 4: P–E (polarization-electric field) hysteresis loops of pure and Sm-doped CaTiO3

Sample	Remnant Polarization in μC/cm²	Coercive Field in kV/cm
Pure $CaTiO_3$	0.28	3.2
Sm doped $CaTiO_3$	0.56	4.1

Table 2: **Ferroelectric results of Samples**

In results, presented in the table 2, the pure $CaTiO_3$ sample exhibited a relatively weak ferroelectricity due to its inherent centrosymmetric structure and limited domain switching. In contrast, Sm-doped $CaTiO_3$ demonstrated a significant improvement. The enhancement in Pr suggests better ferroelectric domain alignment and polarization retention, which can be attributed to the substitution of Ca^{2+} by Sm^{3+} at the A-site of the perovskite lattice.

These findings confirm that Sm doping not only stabilizes the ferroelectric phase but also improves the functional ferroelectric response of $CaTiO_3$, making it more suitable for memory and actuator applications.

4. Conclusion:

Pure and Sm-doped $CaTiO_3$ samples were successfully synthesized by the solid-state reaction route. SEM revealed that Sm doping significantly altered the surface morphology, increasing grain size and surface roughness. EDX confirmed successful doping. These results suggest that Sm-doped $CaTiO_3$ is promising for advanced functional materials due to its enhanced microstructural features. Sm doping significantly improves the dielectric constant and ferroelectric response of $CaTiO_3$. These improvements are associated with lattice modifications and enhanced grain boundary characteristics. The results indicate that Sm-doped $CaTiO_3$ holds promise for advanced electronic applications.

5. References:

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