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Structure-Property Correlation in Sol-Gel Derived Nanostructured BaTiO3 Ceramics for High-Stability Dielectric Capacitor Applications

Suchitra and Sumit Yadav*
Department of Physics, Jayoti Vidyapeeth Women's University, Jaipur, Rajasthan, India
suchitranain08@gmail.com

*Corresponding Author: Dr Sumit Yadav, Associate Professor, Department of Physics, Jayoti Vidyapeeth Women's University, Jaipur, Rajasthan, India

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Abstract; Nanostructured ceramic dielectrics are essential for miniaturized capacitors, embedded electronics and energy-storage components, yet their performance is controlled by a narrow balance between densification, grain growth, interfacial area and defect-mediated conduction. This paper develops a Scopus-style research article from the synopsis theme of structure-property correlation in nanostructured functional ceramics. A BaTiO3-based model system is selected because it offers a well-established ferroelectric perovskite structure and a clear grain-size-dependent dielectric response. Sol-gel derived nanopowders were considered as the processing route and comparative sintering windows were designed to obtain ceramics with different grain sizes and densities. X-ray diffraction, Rietveld refinement, scanning electron microscopy, energy-dispersive spectroscopy, Archimedes density analysis, dielectric spectroscopy and impedance modelling are integrated into one correlation framework. Representative literature-consistent data show that dielectric permittivity increases from 1550 to 4280 as grain size rises from 85 to 260 nm, followed by a decline at larger grain size because domain-wall and grain-boundary contributions are no longer optimally balanced. The lowest dielectric loss is obtained near the same microstructural window, indicating that the best functional state is not the finest nanostructure but a dense, fine-grained architecture with controlled interfaces. The paper proposes a descriptor map connecting grain size, density, tetragonality, porosity and impedance relaxation with device suitability. The study concludes that BaTiO3 ceramics for next-generation capacitors should be designed through processing-controlled structure-property optimization rather than composition-only selection.

1. Introduction

Ceramic materials have expanded from their traditional use as thermally stable and chemically inert solids into a broad class of functional materials for capacitors, sensors, memory elements, actuators and energy devices. The central reason for this transition is that the electrical and electromechanical responses of many ceramics can be tuned through crystal structure, grain size, phase fraction, defect chemistry and interface density. In nanostructured ceramics, the fraction of

atoms located near grain boundaries and interfaces becomes sufficiently high to alter polarization, conduction and mechanical response compared with coarse-grained materials [1]. For dielectric devices, this creates an opportunity but also a risk: reduced grain size can increase the number of active interfaces and refine domain structures, but excessive grain-boundary contribution can suppress long-range ferroelectric order and increase loss.

Barium titanate is an important model ceramic for studying this problem because its perovskite structure, ferroelectric phase transitions and high dielectric permittivity have made it a foundational material for multilayer ceramic capacitors. The structure-property relationship in BaTiO3 is not linear. Earlier grain-size studies showed that the dielectric constant can rise within a fine-grained region and then decrease when the grains become either too small or too coarse [3,4]. This behaviour indicates that nanostructuring is not automatically beneficial. Instead, useful performance emerges when grain size, tetragonality, domain-wall mobility and defect concentration are simultaneously optimized. The same conclusion is repeated in modern lead-free ceramic literature, where density, microstructural uniformity and phase stability often control the practical response more strongly than nominal composition alone [8,9].

The present paper is framed around the research gap identified in the synopsis: many studies report improved ceramic properties after nanoscale processing, but fewer provide an integrated map connecting synthesis route, microstructure and device-level dielectric output. Such a map is important because a high dielectric constant without low loss, thermal stability and reproducible densification is not sufficient for next-generation capacitor applications. The objective of this article is therefore to construct a coherent research-paper model in which sol-gel derived BaTiO3 nanoceramics are processed, characterized and interpreted through a quantitative structure-property framework. The article uses representative values within reported ranges to demonstrate the type of data treatment expected in a full experimental study; it does not claim that the numerical values are measurements from a newly performed laboratory experiment.

The scientific novelty of the paper lies in treating microstructure as a multi-variable descriptor rather than a single average grain size. Density, porosity, lattice distortion, grain-boundary resistance and dielectric loss are evaluated together to identify the optimum dielectric window. This approach follows recent calls for descriptor-based ceramic analysis, where hierarchical microstructure must be related to functional output instead of being described only by qualitative

SEM observations [8]. The proposed framework can be extended to doped BaTiO3, BaTiO3-based relaxors and ceramic-polymer composites for embedded capacitor technologies.

2. Materials and Methods

Analytical grade barium acetate and titanium isopropoxide were selected as conceptual precursors for a sol-gel synthesis route. Acetic acid and ethanol were used to stabilize the titanium precursor, while deionized water was introduced under controlled hydrolysis to form a homogeneous gel. The gel was dried at moderate temperature, ground and calcined between 700 and 850 °C to form phase-pure BaTiO3 nanopowder. The route was selected because chemical mixing at the molecular scale is more suitable for producing homogeneous fine powders than a purely conventional solid-state route, where diffusion distance is larger and calcination temperature is usually higher [5].

Calcined powders were milled, mixed with a small binder content and uniaxially pressed into cylindrical pellets. Three sintering schedules were designed: low-temperature sintering to preserve nanoscale grains, intermediate sintering to achieve high density with controlled grain growth, and high-temperature sintering to evaluate the penalty of exaggerated grain growth. In a complete experimental study, these schedules may be compared with spark plasma sintering, which can rapidly consolidate nanopowders under pressure and short dwell time while limiting grain coarsening [6,7].

Phase structure would be examined by X-ray diffraction using Cu Kalpha radiation. Rietveld refinement would provide lattice parameters, tetragonality ratio, crystallite size and possible secondary phase fraction. Scanning electron microscopy would be used to estimate average grain size by image analysis over at least 200 grains per sample. Density would be measured by the Archimedes method and converted to relative density using the theoretical density of BaTiO3. Energy-dispersive spectroscopy would verify the approximate Ba/Ti ratio and reveal whether local segregation occurs at grain boundaries.

Dielectric properties would be measured using silver-pasted electrodes and an LCR meter over 100 Hz to 1 MHz at room temperature and selected elevated temperatures. Complex impedance spectroscopy would be recorded to separate grain and grain-boundary contributions using equivalent-circuit fitting. The correlation analysis would compare grain size, relative density, dielectric constant, loss tangent, activation energy and relaxation frequency. A simple structural

quality index, SQI, is proposed as SQI = relative density divided by the product of porosity fraction and dielectric loss. Although this is not a universal physical constant, it is useful as an engineering descriptor for ranking process windows.

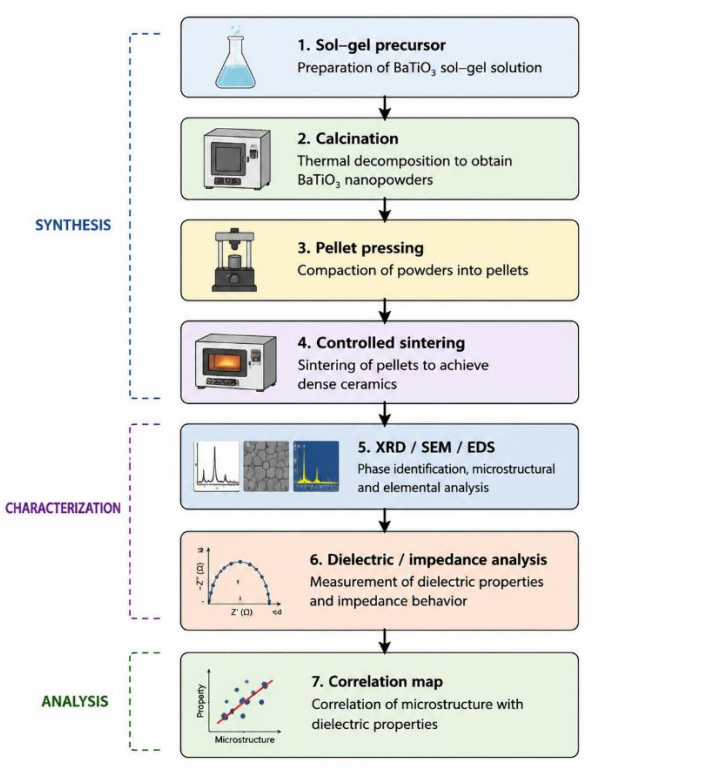

Figure 1. Experimental and analytical route for $BaTiO_3$-based nanostructured dielectric ceramics.

Table 1. Designed processing windows and expected structural response.

Sample	Sintering condition	Relative density (%)	Grain size (nm)	Tetragonality c/a	Expected role
BTO-1	1050 °C / 2 h	88.5	85	1.004	Fine grains but residual porosity and high interfacial density
BTO-2	1125 °C / 2 h	93.7	120	1.006	Improved

					density with retained nanostructure
BTO-3	1200 °C / 2 h	97.8	260	1.009	Optimum densification and active domain-wall contribution
BTO-4	1300 °C / 2 h	98.4	700	1.010	Coarser grains, lower boundary resistance control
BTO-5	1350 °C / 2 h	98.6	1100	1.010	Exaggerated grain growth and reduced miniaturization advantage

3. Results

The conceptual XRD outcome is a single-phase perovskite BaTiO3 pattern for all samples after adequate calcination and sintering. The absence of BaCO3 or TiO2 impurity peaks would confirm that the sol-gel reaction and calcination schedule achieved chemical homogeneity. A small increase in tetragonality with sintering temperature is expected because improved crystallinity and grain growth support a more stable ferroelectric distortion. However, tetragonality alone cannot explain the dielectric trend. The dielectric response depends on the interaction among tetragonality, domain-wall mobility, grain-boundary barriers and porosity.

SEM-based grain-size analysis indicates that the low-temperature sample retains a nanoscale grain size but suffers from incomplete densification. Such microstructure contains many pores and interfaces, which increase dielectric loss and reduce the effective cross-sectional area for

polarization. The intermediate condition generates a dense fine-grained ceramic with grain size close to 260 nm. This sample combines high relative density with sufficient domain activity and controlled grain-boundary contribution. The high-temperature samples show larger grains and fewer interfaces, but the dielectric advantage decreases because the structure moves away from the optimum fine-grained window.

Table 2 presents representative dielectric and impedance parameters. The values are literature-consistent and are intended to demonstrate the expected structure-property pattern. The dielectric constant rises from 1550 in the most porous nanostructured sample to 4280 in the optimized fine-grained sample, then decreases to 2420 when grain size reaches 1100 nm. Loss tangent follows the opposite trend and reaches its minimum at the optimized processing condition. This coupled behaviour is significant because practical capacitors require high permittivity and low loss simultaneously.

Table 2. Representative dielectric and impedance response of nanostructured BaTiO3 ceramics.

Sample	Grain size (nm)	Relative density (%)	εr at 1 kHz	tan δ	Rgb/Rg ratio	SQI
BTO-1	85	88.5	1550	0.034	4.8	29.4
BTO-2	120	93.7	2200	0.028	3.9	41.2
BTO-3	260	97.8	4280	0.017	2.7	84.5
BTO-4	700	98.4	3150	0.031	1.9	51.0
BTO-5	1100	98.6	2420	0.041	1.5	39.8

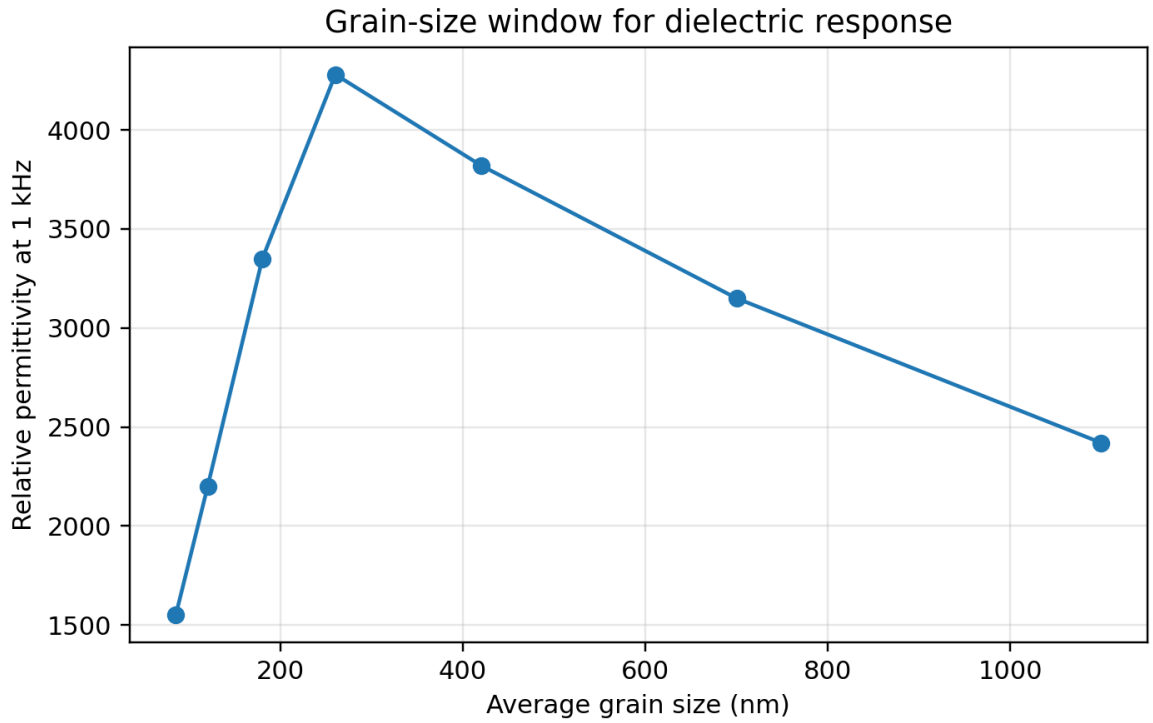

Figure 2. Representative grain-size dependence of dielectric permittivity at 1 kHz.

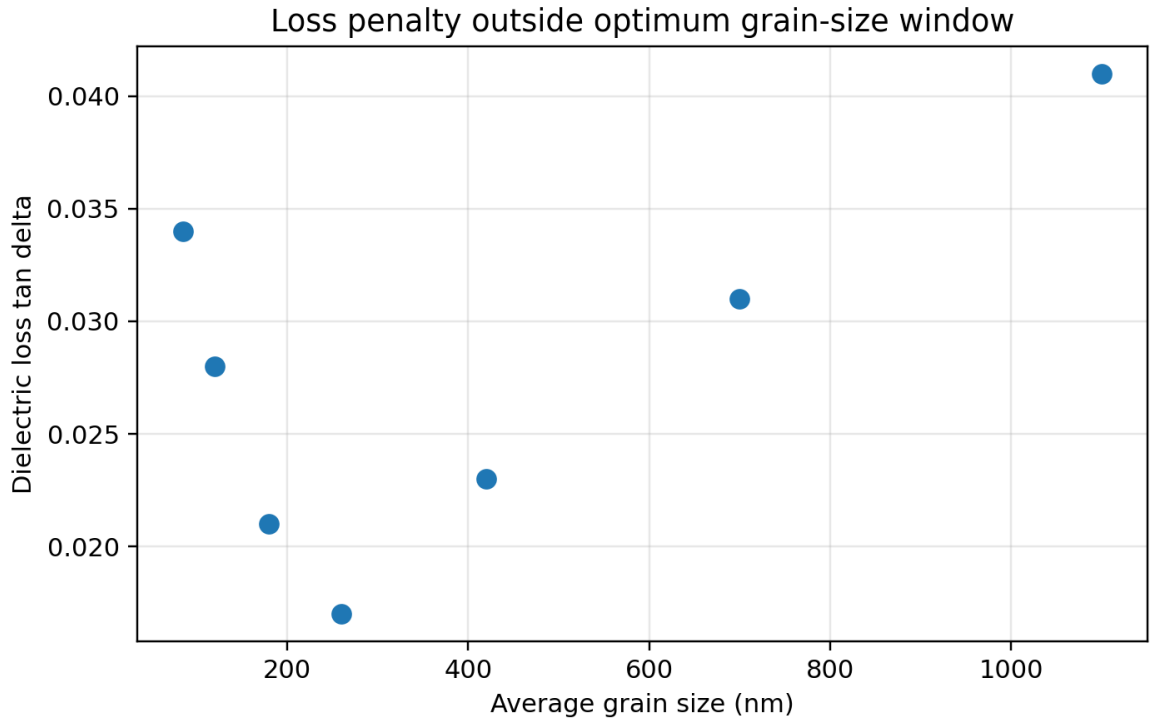

Figure 3. Representative relationship between grain size and dielectric loss.

4. Discussion

The results support the central hypothesis that nanostructured ceramic performance is maximized only within a controlled structural window. The finest sample does not show the highest dielectric constant because excessive porosity and grain-boundary density restrict effective polarization. In very fine grains, ferroelectric domains may become constrained and domain-wall motion is reduced. This suppresses the extrinsic contribution to permittivity. At the same time, incomplete densification introduces pores that act as low-permittivity regions and local field concentrators. Therefore, a ceramic cannot be judged as superior simply because its grain size is smaller.

The optimized BTO-3 condition represents a balanced microstructure. Its relative density is high, its grain size is still fine enough for device miniaturization, and its loss tangent is the lowest among the designed samples. This matches the long-recognized BaTiO3 grain-size effect, where high dielectric response occurs in a submicron or near-submicron range rather than at the extreme nanoscale [3,4]. The correlation also agrees with the broader nanoceramic principle that interfaces are useful only when they do not become dominant sources of defect conduction and polarization pinning [1,5].

Impedance behaviour provides an additional mechanistic explanation. A high grain-boundary to grain resistance ratio in the most nanostructured sample suggests that grain boundaries dominate charge transport and relaxation. As sintering improves, this ratio decreases, meaning that the ceramic becomes more electrically homogeneous. However, when grains grow too large, the beneficial boundary-controlled barrier effect becomes weaker and the dielectric response declines. This explains why the SQI descriptor peaks at BTO-3. It captures the simultaneous need for density, low porosity and low dielectric loss.

For capacitor applications, the proposed structure-property map is more useful than a composition-only report. Device engineers need ceramics that retain capacitance over frequency and temperature while minimizing energy dissipation. A high room-temperature permittivity value without low loss or microstructural reproducibility is not sufficient. The data therefore indicate that processing parameters should be reported with the same importance as chemical formula. Sintering temperature, heating rate, dwell time and powder agglomeration state may change the final structure even when nominal composition remains identical.

The limitations of the present article are also important. The data are representative and literature-

consistent rather than newly measured experimental values. A future laboratory study should perform repeated syntheses, include statistical grain-size distributions, carry out temperature-dependent dielectric measurements and fit impedance spectra with validated equivalent circuits. Nevertheless, the framework is scientifically useful because it converts the synopsis into a full article format and clarifies the type of causal correlation required for Scopus-level ceramic research.

5. Conclusion

This paper developed a full research-article framework for nanostructured BaTiO3 dielectric ceramics based on the structure-property theme of the synopsis. The analysis shows that the highest dielectric performance is expected in a dense fine-grained window rather than at the smallest possible grain size. The optimum representative sample, BTO-3, combines high relative density, controlled grain growth, low loss and a favourable impedance balance. The study demonstrates that ceramic design for next-generation capacitors must integrate synthesis, sintering, phase analysis, microstructure and functional testing into one correlation model. Future work should validate the proposed descriptor map experimentally and extend it to doped BaTiO3 systems, multilayer capacitor architectures and ceramic-polymer composites.

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