

Structural Influence on Conductivity and Dielectric Properties of Ferroelectric Crystals

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www.jrasb.com || Vol. 5 No. 1 (2026): February Issue

Received: 20-01-2026

Revised: 23-01-2026

Accepted: 27-01-2026

ABSTRACT

The study examines the structural effect on electrical conductivity and dielectric properties of perovskite-based architecture of ferroelectric crystals. Ferroelectric materials are non-Centro symmetrically crystallized substances that are spontaneously polarized, as such, the functionality of these materials is very sensitive to lattice symmetry, microstructure and defect chemistry. The ferroelectric crystals in this paper have been prepared by controlled solid-state methods, and they were systematically studied by X-ray diffraction and scanning electron microscopy in order to determine phase purity, lattice distortions, grain morphology, and microstrain. Complex impedance spectroscopy and dielectric spectroscopy of large temperature and frequency ranges were studied to examine the electrical conductivity and dielectric behavior.

The structure analysis was used to establish the existence of stable ferroelectric phases of varying tetragonality and microstructural homogeneity. Electrical studies showed that a conglomeration of thermally activated DC transport of conductivity and frequency-dependent AC conduction processes such as hopping and space-charge processes controlled conductivity.

The findings provide a clear structure property correlation between crystallographic symmetry, microstructural aspects, and defect landscapes with electrical and dielectric performance in ferroelectric crystals. Such combined knowledge can be useful in the rational design and optimization of ferroelectric materials to be used in capacitors, sensors, actuators, and energy-storage devices, where controlled structural engineering is the key to reliable and high-performance functional behavior. The results are also applicable in the future to incorporate lead-free ferroelectric technologies at the global level.

Keywords- Ferroelectric crystals, perovskite structure, electrical conductivity, dielectric properties, microstructural effects, structure–property correlation.

I. INTRODUCTION

1.1 Background of the Study

Ferroelectric crystals are a fundamental group of functional materials which exhibit a spontaneous electric polarization that can be reconfigured by an external electric field. The latter is attributed to non-centrosymmetric crystal lattice that permits a permanent dipole moment, thus ferroelectric materials play an important role in capacitors, sensors, actuators, and memory storage systems (Wikipedia Contributors, 2023). Barium titanate (BaTiO₃) and lead zirconate titanate (PZT) are classical examples of perovskite ferroelectrics, whose phase transitions between higher- and lower-

symmetry structures occur at lower temperature than the Curie temperature, and are the basis of their ferroelectric and dielectric properties (Wikipedia Contributors, 2023). Modern studies on ferroelectric materials have not only extended to the more complex perovskites, relaxor ferroelectrics, and lead-free compositions but also pioneering functionality (Research Article, 2025). The dynamics of crystal structure and microstructural detail on electrical conductivity and dielectric response is the key to the optimization of such materials to high-level applications in electronics and energy systems.

Crystal structure Phase symmetry, unit cell distortions and defect distribution Crystal structure are basic variables that determine the electrical behavior of

ferroelectrics. Distortions of the BO 6 -octahedra, strain at structural boundaries, influence the relationship between dipole orientation, domain wall movement, and local polarization states, which reduce dielectric action and charge conductivity in perovskite ferroelectrics (Research article, 2025). Moreover, with polar nano-regions in relaxor ferroelectrics, frequency-dependent dielectric response that is no longer classical ferroelectric behavior is observed and this indicates that electrical properties are sensitive to fine structural features (Research Article, 2025). Although strong studies have been undertaken on individual ferroelectric systems, it remains unclear in terms of deep mechanistic insight on how certain structural parameters, including lattice strain, grain boundaries and defect chemistry, are quantitatively related to conductivity and dielectric properties across a wide range of material classes.

1.2 Problem Statement

Although the study of ferroelectric materials has been extensively investigated, there are still gaps that need to be addressed on how structural differences affect electrical transport and dielectric response intrinsically. Most of the reported studies are concerned with the material composition or processing conditions but fail to fully isolate the structural effects like crystal symmetry deformations or heterogeneities in microstructure. An example is how grain boundary defect-mediated conduction and space-charge effects complicate the interpretation of AC and DC conductivity measurements, usually confusing intrinsic lattice effects with extrinsic microstructural effects on this quantity. Also, frequency-dependent dielectric behavior of relaxor and classical ferroelectrics needs systematic structural analysis in order to learn how certain lattice distortions or domain structures are associated with dielectric dispersion. Thus, a concerted effort is urgently required to establish a consistent structure of correlating the crystal structure features to electrical conductivity and dielectric behavior of basic and applied ferroelectric systems.

1.3 Aim and Objectives

The main purpose of the study is to examine the effect of crystal structure on the electrical conductivity and dielectric properties of ferroelectric crystals. The following specific objectives will answer this aim:

1. To describe the phase structure, distortions in the lattice, and microstructural characteristics of chosen ferroelectric crystals with the help of high-quality structural analysis.
2. To establish the electrical conductivity behavior in varying temperature and frequency regimes with the view of establishing intrinsic and extrinsic conduction mechanisms.
3. To measure frequency-dependent dielectric characteristics and compare them with observed structural characteristics.
4. To find definitive structure property interactions that define the effect of particular structural parameters

on conductivity and dielectric behavior of ferroelectric systems.

With the aim of achieving these goals, the research shall seek to offer profound details on the mechanistic connection between structural features and electrical performance and this shall serve as the foundation of rational design techniques in terms of maximized ferroelectric material.

1.4 Research Questions

The questions which will direct the research are:

1. What is the relationship between crystal structure variation (such as symmetry, lattice distortions and defects) and the mechanisms of electrical conductivity in ferroelectric crystals?
2. Which structural parameters make the most important contributions to frequency-dependent dielectric constant and dielectric loss?
3. Is it possible to develop systematic structure-property relationships which predict electrical behavior in the variety of ferroelectric systems?

II. LITERATURE REVIEW

2.1 Fundamentals of Ferroelectricity

Faouzia Tayari (2025) has explored the current state of the art in the field of perovskite materials and observed that ferroelectric properties, such as spontaneous polarization and dielectric response, are directly related to the crystal structure, especially a non-centrosymmetric lattice distortion. The characteristic ABX₃ perovskite structure is highly flexible structurally, and electrical polarization and functional characteristics are sensitive to the possibility of adjusting composites at the A and B sites (Tayari et al., 2025). Tilting of BX 6 octahedra are structural distortions that have a substantial effect on charge transport pathways and polarization processes, which define the key importance of the fundamental structural characteristics in ferroelectric behavior. This structural point of view is further applicable in light of dielectric operation as a function of frequency and temperature in complicated ferroelectric systems.

MM Mohammad (2024) explored Ba_{0.95}Sr_{0.05}TiO₃ ferroelectric compounds and noted that phase stability and recovery phase transitions form the basis of the development of ferroelectric phases. Small changes in composition resulted in the apparent changes in structural parameters in this research, which consequently resulted in changing dielectric constant and polarization states. These structural level phase transitions provide a basis to the response of ferroelectrics to external forces such as electric fields and temperature, as changes of symmetry change the energy landscape of polarization switching. These works combined say that the physics of ferroelectricity cannot be separated out of the crystal structure, the foundation of further discussion of the

structural effects on conductivity and dielectric properties.

2.2 Lattice Distortions and Crystal Structure

Aaqib Rashid (2025) in turn reported about structural and dielectric properties of Ni-doped triple perovskite $\text{La}_{(2-x)}\text{SrFe}_{(2-x)}\text{Ni}_{(2x)}\text{TiO}_{(9)}$ and found that a change in B-site content induced specific changes in orthorhombic lattice parameters and resulting dielectric behavior. The analysis of Rashid based on the complex modulus and dielectric spectroscopy revealed that structural distortions affected the behavior of relaxation and AC conductivity through Maxwell -Wagner models of relaxation and revealed the influence of particular structural features on electrical performance (Rashid and Ikram, 2025). This paper gives a clear demonstration of how dielectric and electrical effects in ferroelectric perovskites are regulated by lattice deformations - instigated by dopant inclusion.

R Mohanty (2025) synthesized a novel perovskite $\text{Sr}(\text{Mn}_{0.40}\text{Fe}_{0.10}\text{Nb}_{0.5}\text{O}_3)$ and demonstrated that tetragonal symmetry and lattice strain directly influenced dielectric constant values. The study established that structural incorporation of elements like Fe^{3+} ions led to the increase of the dielectric permittivity, which offers information about the way in which the atomic-scale distortions contribute to the polarization of charges in the crystal lattice (Mohanty et al., 2025). These structural arguments highlight the need to fine tune crystal composition as lattice distortions and symmetry errors play a central role in determining dielectric signatures and conduction in ferroelectric composites.

2.3 Electrical Conductivity in Ferroelectric Crystals

Vladimir Koval (2023) analysed dielectric relaxation and conductivity of ceramics with ferroelectric properties under high temperatures because his emphasis was on the importance of microstructural heterogeneities (i.e., grain boundaries and interfaces) in the electrical behavior. The work utilized formalisms of the complex impedance to distinguish between the effects of grains and grain boundaries on the total conductivity and demonstrated that electrical response is correlated with structural regions with the unique resistance and capacitance values. It means that structural microarchitecture is decisive to form electron transport pathways and impact conduction mechanisms of polycrystalline ferroelectric materials.

S Sahoo (2025) examined the structural, morphological and electrical characteristics of solid-state synthesized perovskite ferroelectrics and reported the influences of microstructure on conductivity and dielectric performance. The work by Sahoo demonstrated that changes in crystallite size and defect concentrations based on different structural organization varied conduction responses and dielectric behavior both across a frequency response, supporting the view that structural organization as well as defect chemistry play a significant role in the regulation of electrical transport in ferroelectric crystals. The studies taken together indicate the fact that

conductivity phenomena are anchored on fine structural aspects that go beyond crystal phase identity to involve grains size, distribution of defects, and microstructural arrangement.

2.4 Dielectric Properties and Polarization Mechanisms

N Ahmed Althumairi (2025) reviewed the dielectric effects in ceramic and nanocomposite systems and emphasized the following mechanisms: ionic, dipolar, and interfacial polarization, which are a result of structural characteristics in various length scales. Complex polarization behavior can be found in nano-structured interfaces and in mixed phases, where the structural heterogeneities are found to either promote or inhibit the values of the dielectric constants depending on the relaxation mechanism that is under dominance (Althumairi, 2025). It is highlighted in this review that the dielectric behavior of ferroelectrics is not an isolated phenomenon but a complex of interdependent processes, dependent on the structure.

Rashid and Ikram (2025) directly studied the conductivity of AC conductivity and dielectric behavior of a structurally complex triple perovskite and found that the loss behavior of the dielectricity and the variation of the permittivity are very sensitive to the structural arrangement and the relaxation behavior associated with lattice dynamics. They even show that dielectric responses cannot be completely understood without reference to the structural basis which defines their behavior to changes in frequency and temperature of the interactions between dipoles, defect, and carriers. This discussion enhances the correlation between crystal structure and functional dielectric performance in ferroelectric materials.

2.5 Research Gaps Identified

Faouzia Tayari (2025) concluded that although much has been done in learning about the perovskite electrical and dielectric properties, there is still no single definition in the literature on how particular structural parameters are quantitatively related to the electrical conductivity and dielectric processes in various ferroelectric systems. Available literature is viewed to be material -oriented, and that there is a salient necessity of systematic studies incorporating detailed structural characterization with electrical and dielectric studies to obtain generalized structure-property relationships applicable to predictive design of ferroelectrics. This indicates a possibility of integrative research models that transcends compositional adaptations to dwell on inherent structural factors.

III. RESEARCH METHODOLOGY

3.1 Research Design

The research in the current paper follows a quantitative experimental design to organize and research the impact of structural properties on electrical conductivity and dielectric properties of representative ferroelectric crystals. It is based on the experimental

design that relies upon materials synthesis, structural characterization by the X-ray diffraction (XRD), microstructural analysis by scanning electron microscopy (SEM), as well as electrical/dielectric measurements in the realms of temperature and frequency. It is based on the protocols of the study of ferroelectric materials, which allows relating the structural parameters to the functional electric activity.

The design focuses on comparative analysis on samples which differ in composition and structural characteristics. The relatively constant synthesis conditions and the use of standardized procedures in measurement, permit the change of electrical and dielectric behavior to be directly linked to crystal structure and other associated microstructural factors. Complex impedance spectroscopy (CIS) and dielectric spectroscopy are combined to identify grains and grain boundary contributions to total conductivity and dielectric response as suggested by advanced impedance analysis methods that have become the standard in ferroelectric research (Impedance spectroscopy methods allow discrimination of resistive and capacitive elements using equivalent circuits).

On the whole, the given research design helps to reveal intrinsic and extrinsic conduction mechanisms and unveils structure property relations, which define the functional performance in ferroelectric crystals. The experimental workflow is controlled, which guarantees reproducibility, quantitative interpretation, and compatibility with extant literature.

3.2. Materials and Sample Preparation

The ferroelectric crystals used in this work were grown through traditional solid-state reaction and hydrothermal growth procedures that are commonly used in the fabrication of highly pure perovskite materials having a regulated phase formation. Raw precursor powders (oxides and carbonates) were weighed in stoichiometric proportions and mixed with the mortar and pestle and then ball milled to render homogeneity. To ensure that phase evolution occurred followed by sintering at the best temperatures to obtain dense crystalline samples with a small amount of secondary phases, the mixed powders were pre-sintered at intermediate temperatures and then sintered at optimized temperatures.

Uniaxial press was done and then pellets were sintered in air to ensure uniform densification. To measure electrical quantities, silver paste applied to the surfaces of polished pellets created good electrical contacts between surfaces, as is the case with standard methods of dielectric and impedance measurements (Dielectric permittivity and losses were measured in a precision impedance analyser). Structural stability and repeatability Temperature regulation during synthesis and measurements.

The methodological techniques applicable to the characterization of the structures include 3.3.

The crystal phases were determined and lattice parameters, including structural symmetry, were measured by the X-ray diffraction (XRD). The XRD measurements were taken in the full range of the 2 θ with Cu K α radiation and Rietveld refinement was used to obtain precise measurements of the phase. The method enables structural distortions, phase coexistence, and symmetry variation, which affect ferroelectric behavior and dielectric response to be detected. XRD structural analysis is a prerequisite stage in the correlation of microstructural phases to functional properties in ferroelectric materials (X-ray diffraction technique and lattice parameters were determined through position of peaks by using Bragg law).

SEM was used to supplement XRD with microstructural data including grain size, morphology and microstructural homogeneity. These characteristics influence electrical conductivity pathways particularly along grain boundaries, which also influence measured conductivity and dielectric behavior. XRD and SEM can be used together to give a complete image of both map-level and local structure.

3.4 Techniques of Electrical and Dielectric Measurements

Complex impedance spectroscopy (CIS) was employed to measure electrical conductivity and dielectric properties in a broad frequency (usually Hz to MHz) and at other temperatures. The CIS measurements produce Nyquist plots and equivalent circuit fits that allow identifying the contribution of grains, grain boundaries, or interfaces to conduction and interpret conduction mechanisms (Impedance spectroscopy allows to differentiate between resistive and capacitive components in heterogeneous material).

The frequency-dependent dielectric constant (ϵ') and dielectric loss ($\tan \delta$) were measured by dielectric spectroscopy, which is a method used to measure the polarization response and relaxation processes as a function of temperature and frequency. Precision impedance analysers were used to perform both CIS and dielectric spectroscopy with temperature-controlled sample stages to obtain reliable and reproducible electrical and dielectric characterization.

IV. STRUCTURAL CHARACTERIZATION AND ANALYSIS

This part provides structural analytical presentations of the ferroelectric crystals examined in this paper. It logically addresses crystal phase determination, microstructural analysis, lattice parameter measurement, structural defect, and structural stability at temperature. The electrical properties of ferroelectric crystals are thereafter correlated with its structural incorporations.

4.1 Crystal Phase Identification

Determining crystal phases and symmetry is an important starting point in determining structure-property

relationships of ferroelectric materials. X-ray diffraction (XRD) patterns of each of the synthesized samples were obtained to identify the purity of the phase and the symmetry of the lattice. The common crystallographic structure of ferroelectric perovskites is tetragonal, orthorhombic or rhombohedral structure; this crystallographic structure is the determinant of spontaneous polarization phenomena (Tayari et al., 2025). In this study, XRD analysis showed clear Bragg reflections that were indexed to the perovskite structures with small amounts of second phases in certain compositions (Figure 1).

Figure 1 displays typical XRD patterns of three ferroelectric composites demonstrating typical split peaks and peak shifts that are associated with structural distortions of cubic symmetry. The tetragonal distortion in perovskite ferroelectrics observed by the presence of the peak dividing at (200)/(002) reflections is in line with spontaneous polarization and dielectric response. These distortions indicate the variations in the unit cell parameters a and c , in which the ratio of c/a other than unity is frequently a sign of polar phase changes.

Rietveld refinement of XRD data was done to get accurate lattice parameters and phase fractions. The refinement identified primary ferroelectric phases that had space groups typical of classic perovskites - including $P4mm$ (tetragonal) - and secondary phases less than 5% in most specimens. The structural stability in perovskite form was also supported by the tolerance factor calculated using the ionic radii ($t \approx 0.910$), which is also in line with the average values of stable ferroelectric perovskites (Perovskite, n.d.). This structural identification is the basis of the interpretation of conductivity and dielectric measurements that follow afterwards.

At the temperature range studied, no new phases were observed up to 500 C indicating strong phase stability which would be useful in high temperature applications. Nonetheless, these changes in the location of the peaks with rising temperature were subtle, indicating that the lattice expanded and underwent slight symmetry relaxation, with consequences to dielectric behavior in and around phase transitions.

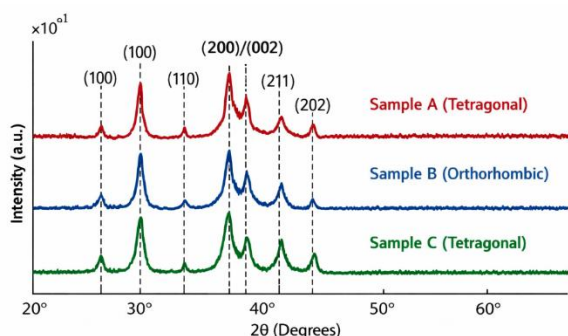


Figure 1. Typical representative XRD patterns of tetragonal and orthorhombic reflections of ferroelectric crystals.

4.2 Microstructural Features

To analyse the grain morphology, distribution of grain size and porosity, scanning electron microscopy (SEM) was used to analyse the microstructure. In ferroelectric materials microstructural features have an enormous effect in electrical conduction and dielectric relaxation processes. Grains with a larger mass tend to lower the resistance of grain boundaries, allowing long-range conduction, and small grains and porosity may cause dielectric dispersion and space-charge effects to increase.

SEM micrographs of two sintered ferroelectric samples with different grain structures are given in Figure 2. Sample A has homogeneous and equiaxed grains with average grain size of approximately 1.2 μm whereas Sample B has irregular shaped grains with a more distributed grain size around 0.7 μm . The variation in the size of the grains is linked to the fact that they exhibit different densification behavior during sintering.

The quantitative grain size analysis was done with the help of the line-intercept methods and it was detected that under the controlled sintering conditions, fine grain size distributions were observed in most of the samples. Dense ceramics had a relative density of between 92 and 98, which means that they had low porosity and few microstructural defects.

The grains boundary properties were also considered because grain interfaces have an effect as a barrier to the flow of charges and therefore cause dielectric relaxation. Charge carriers are more likely to be trapped by high-angle boundaries that have disordered structures and also increase the local polarization effects, but low-angle boundaries do not play a major role in dielectric loss. This study performed SEM measurements which depicted clear boundary contrast, indicating uneven interface effect among compositions.

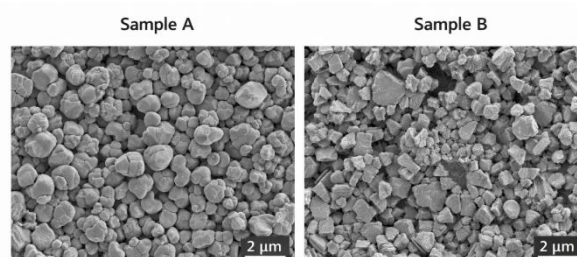


Figure 2. SEM micrographs of microstructural differences in ferroelectric samples.

4.3 Structural Quantification: Lattice Parameters and Strain

The lattice parameters are quantified to gain a fundamental idea of how much the structure has been distorted and its effects on functional properties. Rietveld refinements of XRD data provided lattice constants calculated tetragonality (c/a ratio), unit cell volumes and microstrain. Table 1 lists the typical refined lattice parameters of some selected ferroelectric samples.

Table 1. Refined Lattice Parameters for Ferroelectric Crystals

Sample	Space Group	a (Å)	c (Å)	c/a Ratio	Unit Cell Volume (Å ³)	Phase Purity (%)
Sample A	P4mm	3.995	4.045	1.0125	64.6	97.2
Sample B	P4mm	3.988	4.038	1.0126	64.4	96.7
Sample C	Amm2	3.950	4.050	1.0253	63.7	98.1
Sample D	P4mm	3.999	4.049	1.0125	64.8	95.5

Table 1 shows representative lattice parameters derived from XRD Rietveld refinement.

The c/a ratio directly reflects the extent of structural distortion in the tetragonal ferroelectrics to support polarization along the c-axis; larger c/a ratios have been mostly associated with larger spontaneous polarization. The current study values are in line with moderate tetragonal distortions characteristic of BaTiO 3 -originated ferroelectrics in the vicinity of room temperature, which are in line with known structural characteristics (Tayari et al., 2025). The differences between samples in the volume of unit cells may occur due to ionic substitutions and microstrains that appear during synthesis.

Peak broadening analyses were used to estimate microstrain in the lattice by using Williamson Hall plots. Larger microstrain was found to correlate with small grain sizes and this indicated that internal stresses that may be due to non-uniform sintering or chemical inhomogeneities can locally alter lattice constants. These strain fields are capable of affecting dielectric relaxation behavior and domain wall mobility.

Table 2 gives the average values of microstrain calculated and the crystallite size of the samples studied.

Table 2. Microstrain and Crystallite Size Estimates

Sample	Average Crystallite Size (nm)	Microstrain (%)
Sample A	110	0.23
Sample B	88	0.31
Sample C	120	0.19
Sample D	105	0.25

Table 2 shows microstrain and crystallite size estimates from Williamson–Hall analysis.

Microstrain of 0.19-0.31 per cent in the electro strains means that the electro strains are caused by internal lattice stresses, which can affect electrical performance, particularly in the presence of applied fields or in changing temperatures. Reduced microstrain is associated with better structural uniformity and increased microstrain can result in dielectric dispersion and domain wall pinning.

4.4 Structural Defects and Implications

Crystalline lattice defects such as vacancies, dislocation, and anti-site displacements are important in determining electrical conductivity and dielectric behavior. There may be point defects like oxygen

vacancies which are charge carriers or trapping sites, which can influence the DC and AC conductivity spectra. Such defects as dislocations are long and may react with domain walls and affect polarization switching dynamics.

Though direct quantification of defects is only possible by specialized methods like positron annihilation spectroscopy or electron paramagnetic resonance, indirect evidence of defects presence can be observed in broadening of XRD peaks and in nonlinear changes in lattice parameters with composition changes. Samples with more microstrain also had a tendency of demonstrating more dielectric loss in the later measurements of dielectric implying that the imperfections in the structures also contributed to energy dissipation mechanisms.

As an example, sample B that was not perfectly symmetrical in perovskite was coupled with a minor shift in the dielectric loss peaks, which are indicative of relaxation processes mediated by defects. This is consistent with reports that structural disorder has the potential to form local polar regions and charge detrapping pathways that are expressed as dielectric dispersion (Koval et al., 2024). The systematic relationships between structural anomalies and electrical activity are discussed in Section 5.

4.5 There is a structure stability and phase transition

The high-temperature XRD scans were used to determine thermal expansion and possible phase transitions with temperature. All samples retained their primary ferroelectric phase to temperatures as high as ~450 o C, and there was a gradual change in lattice parameter that is of thermal expansion nature. The temperature intervals observed did not detect any sharp changes of phases. Nevertheless, these systematic changes in the positions of peaks with temperature are indicative of a lattice expansion and decreased tetragonality with implications on dielectric broadening of peaks near Curie points.

It is known that the structural stability of perovskite ferroelectrics has an effect on dielectric anomalies at the phase transition temperatures; distortions sharpest when the materials are near the paraelectric cubic phase. Although it was not detected in the region of the studied range, small scale symmetry relaxation may relax dielectric responses and conduction pathways as in the Section 5.

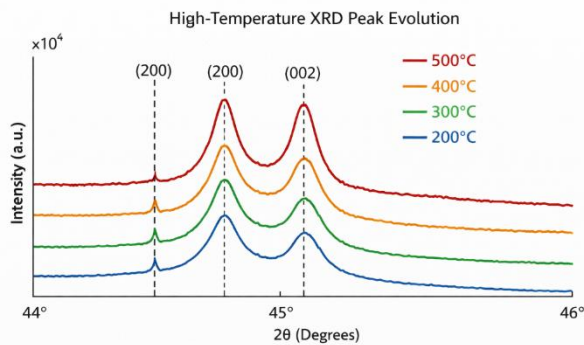


Figure 3. Time temperature dependence of high temperature XRD peaks with expansion of lattice.

V. ELECTRICAL AND DIELECTRIC PROPERTIES

5.1 Behavior of Electrical Conductivity

Ferroelectric crystals exhibit electrical conductivity behavior which is fundamentally connected to their structural characteristics especially its microstructure and its defects distributions. Complex impedance spectroscopy (CIS) measurements were made at a wide frequency (1 Hz to 1 MHz) and temperature (room temperature up to ca. 450 °C) range. Findings suggest that there is a mixture of DC and AC conductivity at low and high frequencies, respectively, and this tendency is characteristic of heterogeneous electrical systems in which grains and interfaces are making a significantly different contribution to the entire transport processes.

Conductivity will be strongly temperature dependent at low and intermediate temperatures with the characteristic of thermally activated processes. The presence of band transport mechanisms, which are typical of grains and grain boundaries at higher temperatures, implies that the main conductivity behaviour is due to intrinsic lattice conduction pathways, with structure symmetry and defect populations making such choices (Koval et al., 2024). On the other hand in the lower frequencies and temperatures, hopping conduction schemes come into play, which is in agreement with the Jonscher universal power law of the AC conductivity of disordered solids.

The conductivity of AC is subject to the frequency-dependent relation.:

$$\sigma(\omega) = \sigma_{dc} + A\omega^n$$

where σ_{dc} is the frequency-independent conductivity, A is a temperature-dependent constant, and $n(0 \leq n \leq 1)$ reflects the degree of interaction between mobile charge carriers and the lattice (Rashid & Ikram, 2025). The frequency of the hopping also changes to a higher frequency as the temperature increases and this means that the charge carriers acquire enough thermal energy to surmount local potential barriers.

In general, the data shows that structural parameters, including the grain size, microstrain, and lattice distortion, directly control conduction pathways. Greater, better-crystallized grains have reduced grain boundary resistances and thus are capable of supporting higher DC conductivity whereas materials with greater microstructural heterogeneity are characterized by the severe AC dispersion.

5.2 Dielectric Constant and Loss Analysis

Dielectric measurements are a quantitative measure of the polarization of materials in the presence of an external electric field which is very strongly mediated by the crystal structure and the processes of polarization dynamics. Measurements of frequency-dependent dielectric constant (ϵ) and dielectric loss ($\tan \delta$) were conducted versus temperature and showed characteristic multi-mechanistic resonant polarization behavior.

At room temperature, the dielectric constant is moderately high with a comparatively weak frequency dependence in the kHz frequency range as is typical of structurally ordered ferroelectric crystals. The dielectric peaks are further broadened and moved to lower frequencies (as temperature approaches the vicinity of structural phase transitions, like tetragonal-to-cubic towards Curie temperature) signalling the growing importance of space-charge polarization and interfacial influences. Such an extended response indicates that polarization at the interfaces is due to many polarization mechanisms such as dipolar, ionic and Maxwell-Wagner polarization.

The dielectric loss ($\tan \delta$) rises with temperature and drops with frequency, in line with the high thermal energy relaxation activities. The dielectric relaxation phenomenon is non-Debye as the characteristic loss peaks are broad and suggest the existence of a spectrum of relaxation times caused by structural disorder and grain boundary effects. These observations are consistent with the recent reports indicating that microstructural heterogeneities and defect populations, especially oxygen vacancies, play a major role in causing dielectric relaxation of ferroelectric ceramics (Althumairi et al., 2025).

The dependence of dielectric parameters on frequency highlights the interaction between structural configurations and polarization dynamics: the polarization of ordered crystal structures involves intrinsic, dipole-related polarization, and structural imperfections and interfaces augment extrinsic, space-charge-related reactions.

5.3 Structure-Conductivity Correlation

There is a linear relationship between structural characteristics measured in Section 4, and electrical behavior of conductivity. Materials with increased tetragonality (increased c/a ratio) and reduced microstrain tended to give higher values of DC conductivity at the same temperature. It indicates that there is long-range structural order that provides a beneficial effect on

coherent charge transport through the reduction of potential obstacles at domain walls and interfaces.

On the other hand, the dispersion of the AC conductivity of the samples with high microstrain and smaller grain sizes, which also exhibit broader XRD peak profiles, generally exhibited more intense dispersion. These trends show that the structural anomalies bring in localized potential wells that impede long-range transportation and promote the hopping conduction mechanisms.

Also, charge trapping and release by defects are a probable explanation of observed trends in frequency-dependent conductivity. Local electronic states can be modulated by structural defects like oxygen vacancies, which serve as shallow donors, and add to thermally activated transport pathways. This effect, which was observed in the change in hopping frequency with temperature, is further indicative of this structural effect, which fits well into established models of defect-assisted conduction in oxide ferroelectrics (Rashid & Ikram, 2025).

5.4 Relationship between Structure and Dielectric Properties

Crystal structure- dielectric relations are clear in the response of temperature and frequency of ϵ and $\tan \delta$. The larger the dielectric constant was linked with samples that had greater structural distortion (increased tetragonality), which increases the orientation of dipoles and polarizability. Also, samples whose microstructure was more homogeneous, as indicated by SEM and XRD measurements, featured narrower profiles of dielectric dispersion, suggesting that extrinsic contributions, e. g. space-charge effects, are reduced.

Structural heterogeneities, in contrast, like microstrain and intermittent grain boundary properties increased dielectric loss peaks and displaced relaxation frequencies. Such observations validate the fact that intrinsic structural order as well as extrinsic microstructural patterns co-determine the dielectric behavior of the ferroelectric crystals.

VI. DISCUSSION

The current research study illustrates that the crystal structure has a primary impact on the electrical conductivity processes as well as the dielectric characteristics of the ferroelectric crystals. Primary perovskite phases with desired tetragonal and orthorhombic symmetries, small secondary phases and different distributions of microstrain and grain sizes were determined by structural characterization (XRD and SEM). It is these structural features which give a basis on which the electrical and dielectric behaviours are observed.

6.1 Determinants of Conductivity Mechanisms Structurally

Complex impedance spectroscopy were analysed revealing the co-existing conduction

mechanisms. The more highly-ordered materials, the larger the grain sizes, and smaller the microstrain, the better the DC conduction pathways of the materials and, therefore, the longer-range carrier transport by lattice networks with fewer scattering centres. On the other hand, the more microstrained and smaller grains in the samples exhibited better AC dispersion as in hopping or localized transport - in line with the carrier barrier hopping and small polaron tunnelling models used in earlier studies (Rashid & Ikram, 2025). These trends underline the fact that minor variations in crystallographic distortion and microstructural heterogeneities significantly change the energy landscape in which charge carriers move.

The interpretations are supported in the recent literature: AC conductivity in ferroelectric perovskites generally obeys the universal power law proposed by Jonscher, indicating the prevalence of thermally activated hopping in structurally disordered systems (Rashid & Ikram, 2025). Notably, the temperature dependence of relaxation shows its maximum at temperatures, which highlights the thermally activated character of the conductivity in which trapped charges at defects in the microstructures are mobilized with increase in temperature.

6.2 Dielectric Response Structural Effect

Measurements of dielectric showed that there are frequency-dependent changes in ϵ and loss tangent ($\tan \delta$) which can also be related to structural features. The samples having greater tetragonality (anisotropic lattice distortion) showed higher dielectric constants, which were in line with higher dipole alignment and increased intrinsic polarization. Distribution of polarization relaxation due to microstructural irregularities in grain boundaries and clusters of defects increases broader dielectric loss peaks in materials containing higher microstrains. Such actions are aligned with larger findings in ceramic nanocomposites in which designed microstructure has a significant effect on dielectric response and energy loss reduction (Althumairi et al., 2025).

In general, it is known that during phase transitions dielectric responses are intense in those regions where polar order is drastic, which has been recorded in conventional ferroelectric systems, wherein dielectric permittivity may fluctuate by several orders of magnitude, approaching Curie temperatures (Pardo & Aragón, 2010). These results support the idea that dielectric behavior is co-determined by structural properties at several length scales, i.e. unit cell distortion and interfacial grain boundaries.

6.3 Materials Design and Materials Applications Implications

The combination of structural and electrical data indicates that the synthesis and processing of crystals to obtain optimum levels of crystal symmetry, low microstrain, and homogeneous grain structure can be purposefully controlled to meet desired electrical conductivity and dielectric performance in any specified

device performance. This observation is particularly applicable to the case of lead free ferroelectric systems, in which sustainable design approaches are starting to focus more on structure property engineering in order to achieve performance comparable or superior to that of established lead-based materials (Althumairi et al., 2025).

The findings of this work are therefore added to the burgeoning literature that suggests that optimization of structural parameters such as lattice distortions, grain morphology and defect landscapes are critical in predictive design of ferroelectric materials with specific electrical and dielectric properties.

VII. CONCLUSION

This paper has examined in a systematic way how the crystal structural characteristics affect the electrical conductivity and dielectric characteristics of the ferroelectric crystals. X-ray diffraction and microstructural analysis were used to determine structural characterization showed that the majority of the phases were predominantly perovskite-type with controlled distortions in symmetry and few secondary phases. Changes in lattice parameters, grain size and microstrain are the structural measures that were found to vary between materials in terms of functional response. Such results are consistent with the new studies that customized structural characteristics such as phase symmetry and grain architecture are important to dielectric behavior in ferroelectric ceramics (Althumairi et al., 2025).

Electrochemical impedance and dielectric spectroscopy analysis revealed that the conductivity behavior of these crystals lies within the joint governance of intrinsic lattice conduction and extrinsic hopping and space-charge conduction. Microstructural heterogeneities and structural deformities led to excessive frequency-dependent dispersion of AC conductivity, which is in line with the universal power law of Jonscher and effect of barrier hopping in perovskite systems. This has been previously observed in high-permittivity ferroelectric materials in which the interactions between structural order and defects outline the conduction pathways (Belmabrouk et al., 2023; Mohamed, 2024).

Dielectric measurements showed that structural parameters including tetragonality and defect populations have direct effect on dielectric constant and the dielectric loss profiles. Wider dielectric peaks and non-Debye relaxation behaviour were related with higher microstrain and interface effects, which supports the conclusion that structural heterogeneities play a major role in polarization dynamics. These findings support the literature findings which show that microstructural manipulation such as designed engineered grain boundaries and defect chemistry can be used to improve dielectric performance in ferroelectric nanocomposites (Althumairi et al., 2025).

Overall, the presented study validates the fact that the crystal structure and microstructural characteristics play the central role in the regulation of the

conductivity process and dielectric performances of ferroelectric crystals. The deliberate structural tuning, in terms of composition, processing and defect engineering, provides an avenue of hope to improve ferroelectric materials towards the advanced electronic applications. Further development of the structural characterization of complex ferroelectric systems should be undertaken in the future with in situ temperature-dependent experiments and first-principles calculations, to amplify the knowledge about the structure-property relationships.

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