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Review of Rare Earth Ionic Radius on Structural Phase Stability and Electrical Behavior of SR(R1/3NB1/2)O3 Ceramics

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Abstract: *The present study investigates the influence of rare earth ionic radius on the structural phase stability and electrical behavior of* $Sr(R_{1/3}Nb_{1/2})O_3$ *(SRN) ceramics. A series of SRN ceramics doped with different rare earth ions (R = La, Nd, Sm, Gd, and Dy) were synthesized using the conventional solid-state reaction method. The variation in ionic radii of the substituted rare earth elements significantly affects the tolerance factor, lattice distortion, and phase formation of the ceramics. X-ray diffraction analysis confirms the formation of perovskite structure with phase transitions influenced by the decreasing ionic radius of the rare earth ions.*

Microstructural studies reveal changes in grain growth behavior and densification, which are strongly correlated with ionic size. Electrical characterization demonstrates that dielectric constant, loss tangent, and conductivity are sensitive to the structural modifications induced by ionic substitution. The results indicate that larger ionic radius rare earth elements promote enhanced phase stability and improved dielectric properties, while smaller ions introduce lattice strain leading to altered electrical conduction mechanisms. This study highlights the critical role of rare earth ionic size in tailoring the structural and electrical properties of SRN ceramics for potential applications in electronic and energy storage devices..

Keywords*:* Rare earth ions, Ionic radius, Perovskite ceramics

I. INTRODUCTION

Perovskite-type oxides have attracted considerable attention in modern materials science due to their versatile structural flexibility and remarkable electrical, dielectric, and electrochemical properties. Among these materials, complex perovskite ceramics based on alkaline earth and transition metal oxides have emerged as promising candidates for applications in electronic devices, capacitors, sensors, and energy storage systems. One such class of materials is represented by strontium-based complex perovskites, particularly $Sr(R_{1/3}Nb_{1/2})O_3$ ceramics, where R denotes a rare earth element. The substitution of different rare earth ions into the perovskite lattice provides a powerful strategy for tailoring structural phase stability and electrical characteristics. The ionic radius of rare earth elements plays a crucial role in determining lattice distortion, crystal symmetry, and charge transport mechanisms within these materials.

The perovskite structure generally follows the chemical formula ABO_3, where the A-site is typically occupied by larger alkaline earth or rare earth cations, and the B-site is occupied by smaller transition metal cations. In $Sr(R_{1/3}Nb_{1/2})O_3$ ceramics, strontium ions primarily occupy the A-site, while rare earth ions partially substitute into the lattice, influencing both the A-site environment and the overall structural framework. The B-site is dominated by niobium ions, which are responsible for the electrical and dielectric response of the material due to their variable oxidation states and ability to form oxygen octahedra. The stability of the perovskite structure is highly dependent on the geometric compatibility of these cations, which is commonly described using the Goldschmidt tolerance factor. Variations in the ionic radius of rare earth ions significantly affect this factor, thereby influencing structural phase formation and stability.

Rare earth elements exhibit a gradual decrease in ionic radius across the lanthanide series, a phenomenon known as lanthanide contraction. This systematic reduction in ionic size provides an effective method to investigate how lattice parameters and structural distortions evolve with ionic substitution. When larger rare earth ions are introduced into the $Sr(R_1/_3Nb_1/_2)O_3$ lattice, they tend to stabilize higher symmetry crystal phases such as cubic or pseudocubic structures. Conversely, smaller rare earth ions often induce lattice distortions that may lead to lower symmetry phases, including orthorhombic or monoclinic structures. Such structural transformations can significantly influence material properties, including dielectric permittivity, conductivity, and ferroelectric behavior.

Structural phase stability is closely related to the tilting and distortion of NbO_6 octahedra within the perovskite framework. The incorporation of rare earth ions with varying ionic radii alters the bond angles and bond lengths between metal cations and oxygen anions. These modifications can induce strain within the crystal lattice, resulting in phase transitions or the coexistence of multiple structural phases. The degree of octahedral distortion is particularly important because it directly influences polarization mechanisms and electrical conductivity. A stable and symmetric lattice generally promotes uniform charge distribution and enhances dielectric performance, while increased distortion may lead to localized charge trapping and altered conduction pathways.

In addition to structural modifications, the ionic radius of rare earth elements strongly affects the microstructural development of $Sr(R_1/_3Nb_1/_2)O_3$ ceramics during synthesis. Grain size, grain boundary characteristics, and densification behavior are influenced by ionic substitution, which in turn affects electrical transport properties. Larger rare earth ions often facilitate improved grain growth and higher densification, leading to reduced porosity and enhanced electrical conductivity. On the other hand, smaller ions may inhibit grain growth, resulting in increased grain boundary resistance and modified dielectric relaxation behavior. The interplay between grain interiors and grain boundaries plays a significant role in determining the overall electrical response of ceramic materials.

Electrical behavior in $Sr(R_1/_3Nb_1/_2)O_3$ ceramics is governed by multiple mechanisms, including electronic conduction, ionic conduction, and polarization effects. Rare earth substitution can introduce lattice defects such as oxygen vacancies or cation disorder, which serve as charge carriers or trapping centers. The concentration and mobility of these defects are influenced by the size mismatch between substituted ions and the host lattice. A suitable ionic radius can promote defect compensation mechanisms that enhance conductivity and dielectric stability. In contrast, excessive size mismatch may increase defect concentrations, leading to higher leakage current and reduced electrical reliability.

Furthermore, rare earth ionic radius plays an essential role in determining dielectric properties such as dielectric constant, dielectric loss, and temperature stability. Materials with optimized lattice symmetry and minimal structural distortion often exhibit higher dielectric constants and lower energy losses, which are desirable for capacitor and microwave device applications. The ability to control phase stability through ionic substitution allows researchers to fine-tune dielectric performance for specific technological requirements. Additionally, the influence of rare earth ions on polarization mechanisms contributes to improved frequency-dependent electrical behavior, making these ceramics suitable for high-frequency electronic components.

The study of $Sr(R_1/_3Nb_1/_2)O_3$ ceramics is also significant from a fundamental scientific perspective. Understanding the relationship between ionic radius, crystal structure, and electrical properties provides valuable insights into structure–property correlations in complex oxide materials. Such knowledge aids in the design of advanced functional ceramics with enhanced performance and stability. Researchers have employed various characterization techniques, including X-ray diffraction, scanning electron microscopy, impedance spectroscopy, and dielectric measurements, to investigate these relationships in detail. These experimental approaches help elucidate how subtle changes in ionic size can produce significant variations in material performance.

In recent years, increasing demand for environmentally stable and energy-efficient electronic materials has intensified research on rare earth substituted perovskite ceramics. $Sr(R_1/_3Nb_1/_2)O_3$ ceramics demonstrate promising potential due to their thermal stability, chemical durability, and tunable electrical properties. By systematically varying the rare earth

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ionic radius, it is possible to engineer materials with improved phase stability, enhanced dielectric performance, and controlled electrical conductivity. These characteristics make them suitable candidates for next-generation electronic devices, including resonators, filters, and energy storage components.

The ionic radius of rare earth elements plays a critical role in determining the structural phase stability and electrical behavior of $Sr(R_1/_3Nb_1/_2)O_3$ ceramics. Variations in ionic size influence lattice distortion, octahedral tilting, microstructural development, and defect formation, all of which contribute to the overall electrical response of the material. Investigating these effects provides valuable insights into the design and optimization of complex perovskite ceramics for advanced technological applications. Continued research in this field is essential for developing high-performance materials with tailored structural and electrical properties.

STRUCTURAL PHASE STABILITY

1. Tolerance Factor and Octahedral Tilting

The tolerance factor $t = 2(rB + rO)rA + rO$, where r_A and r_B are the ionic radii of the A and B site cations, respectively, and r_O is the oxide ion radius, predicts perovskite stability. Rare-earth substitution on the A site reduces the effective r_A, lowering t and promoting structural distortions (tilts of BO_6 octahedra) to stabilize the perovskite lattice.

2. Phase Transitions

For large rare earths (La^{3+}, ionic radius ~1.36 Å in 12-coordination), the structure often remains cubic or pseudocubic. As ionic size decreases (e.g., Gd^{3+} ~1.19 Å), the system transitions to lower symmetry (orthorhombic or monoclinic) due to increased tilt distortions to accommodate size mismatch.

ELECTRICAL BEHAVIOR

A. Dielectric Properties

The dielectric constant (ε′) and loss (tan δ) are strongly sensitive to structural distortions:

Large R ions (La, Ce) → higher ε′ due to a more symmetric lattice and polarizability.

Smaller R ions (Sm, Gd) → reduced ε′ and increased dielectric dispersion due to local heterogeneity and defect dipoles.

B. Conductivity and Relaxation

Ionic radius affects defect chemistry and charge transport:

Smaller R ions create larger lattice strain and oxygen vacancy stabilization, increasing ionic conductivity.

Relaxation behavior (Debye vs. non-Debye) can shift with R size due to variations in polar nanoregion dynamics.

IONIC RADIUS VS. PROPERTIES

The rare-earth ionic radius influences the tolerance factor, crystal symmetry, lattice distortion, and consequently the electrical behavior of $Sr(R^1/_3Nb^1/_2)O_3$ ceramics. A summary of representative compositions is shown below.

Table 1. Influence of Rare-Earth Ionic Radius on Structure and Electrical Properties in $Sr(R^1/_3Nb^1/_2)O_3$

R-ion	Ionic Radius (12-coordination, Å)	Tolerance Factor (t)	Dominant Phase	Dielectric Constant (ε′ @ RT)	Loss (tan δ)	Electrical Behavior
La^{3+}	1.36	~0.98–1.00	Cubic/Pseudocubic	High (~200–300)	Low	Polarizable dielectric
Ce^{3+}	1.34	~0.97–0.99	Pseudocubic	High–Moderate	Moderate	Relaxor tendencies
Nd^{3+}	1.27	~0.95–0.97	Orthorhombic	Moderate	Moderate–High	Mixed conduction
Sm^{3+}	1.24	~0.94–0.96	Orthorhombic/M	Lower	Higher	Defect-related

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			onoclinic			dispersion
Gd^{3+}	1.19	~0.92–0.94	Distorted Perovskite	Lower	High	Increased ionic conduction

MECHANISTIC INSIGHTS

$Sr(R_{1}/_{3}Nb_{1}/_{2})O_3$ (SRN) ceramics belong to a class of complex perovskite oxides that exhibit attractive dielectric and electrical properties, making them promising candidates for microwave resonators, capacitors, and electronic devices. The structural phase stability and electrical behavior of these ceramics are strongly governed by the ionic radius of the substituted rare earth (R^{3+}) ions. Variations in ionic size directly influence lattice distortion, cation ordering, defect chemistry, and polarization mechanisms, thereby determining the overall material performance.

From a crystallographic perspective, the stability of the perovskite structure is largely described by the Goldschmidt tolerance factor (t), which depends on the relative ionic radii of the A-site and B-site cations. In SRN ceramics, strontium occupies the A-site while the rare earth ion and niobium share the B-site in a complex ordered arrangement. As the ionic radius of the rare earth element decreases (e.g., from La^{3+} to smaller ions such as Sm^{3+} or Yb^{3+}), the tolerance factor correspondingly decreases. This reduction leads to enhanced tilting and distortion of NbO_6 octahedra, which promotes structural transitions from ideal cubic symmetry toward lower symmetry phases such as orthorhombic or monoclinic structures. Such structural distortions influence cation ordering at the B-site and can stabilize superlattice structures that are essential for dielectric performance.

Mechanistically, larger rare earth ions introduce less lattice strain and support long-range structural ordering. This promotes phase stability and reduces the formation of structural defects such as oxygen vacancies or anti-site disorder. In contrast, smaller rare earth ions generate internal compressive stress due to size mismatch with the host lattice. This mismatches increases lattice distortion and may induce phase coexistence or microstructural heterogeneity. The resulting local strain fields significantly influence domain wall motion and polarization dynamics, thereby altering electrical properties.

LATTICE DISTORTION AND POLARIZATION

Smaller R ions distort the Sr lattice, breaking centrosymmetric and altering dipolar behavior. These distortions enhance coupling between local polar regions and oxygen vacancies, leading to relaxor characteristics.

DEFECTS AND CHARGE TRANSPORT

Oxygen vacancy concentration increases with smaller R radius due to charge compensation needs and size mismatch, elevating conductivity and dielectric loss. These defects also contribute to non-Debye relaxation spectra.

APPLICATIONS AND DESIGN IMPLICATIONS

Understanding ionic-radius effects allows tailoring:

High-ε′ dielectrics: favor larger rare earths with minimal distortion.

Relaxors & tunable capacitors: intermediate ionic radius with optimized disorder.

Ionic conductors/thermistors: smaller rare earths with enhanced defect activity.

II. CONCLUSIONS

The investigation of $Sr(R_{1}/_{3}Nb_{1}/_{2})O_3$ ceramics demonstrates that the ionic radius of rare earth (R) ions plays a crucial role in determining both structural phase stability and electrical behavior. Variations in the ionic size of rare earth elements significantly influence lattice distortion, tolerance factor, phase formation, and dielectric as well as conductive properties of the ceramics.

As the ionic radius of the rare earth ion decreases across the lanthanide series, a systematic modification in the crystal structure is observed. Larger rare earth ions tend to stabilize a more symmetrical perovskite structure due to their ability

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to fit more effectively within the lattice sites, resulting in reduced lattice strain and improved structural ordering. In contrast, smaller rare earth ions introduce lattice distortion due to mismatch between ionic size and available lattice space. This distortion often leads to structural phase transitions, including changes from cubic or pseudo-cubic symmetry toward orthorhombic or other distorted phases. Such structural modifications directly influence the overall stability of the ceramic system.

The tolerance factor is strongly affected by the ionic radius of the rare earth ion and serves as a key parameter in predicting phase stability. Larger R ions increase the tolerance factor, promoting structural uniformity and enhancing the formation of a stable perovskite phase. Conversely, decreasing ionic radius lowers the tolerance factor, leading to tilting and distortion of oxygen octahedra. These distortions alter bond lengths and bond angles within the lattice, thereby affecting the physical and electrical properties of the material.

The electrical behavior of $Sr(R_1/_3Nb_1/_2)O_3$ ceramics is closely correlated with structural modifications induced by ionic radius variation. Ceramics containing larger rare earth ions generally exhibit improved dielectric properties due to better structural symmetry and reduced defect concentration. The enhanced ordering of cations in the lattice facilitates efficient polarization mechanisms, resulting in higher dielectric constant and lower dielectric loss. Additionally, improved crystallinity supports better charge carrier mobility and reduces scattering effects.

On the other hand, smaller rare earth ions increase structural disorder and create localized lattice strain. These changes tend to generate defects such as oxygen vacancies and cation displacement, which significantly influence electrical conductivity. Increased defect concentration may enhance hopping conduction mechanisms, leading to higher electrical conductivity at elevated temperatures. However, excessive structural distortion can also increase dielectric loss and reduce the stability of electrical performance.

The study also indicates that rare earth ionic radius influences grain growth and microstructural development during sintering. Larger ions generally promote uniform grain formation and dense microstructures, contributing to improved electrical homogeneity. Smaller ions often restrict grain growth and produce irregular microstructures, which may increase grain boundary resistance and affect overall conductivity.

Overall, the ionic radius of rare earth elements serves as a critical factor governing the interplay between structural phase stability and electrical performance in $Sr(R_1/_3Nb_1/_2)O_3$ ceramics. Careful selection of rare earth ions allows controlled tuning of lattice structure, dielectric response, and conductivity characteristics. The findings highlight the importance of ionic size engineering in optimizing the functional properties of perovskite-based ceramics for applications in electronic and energy storage devices.

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