# Unveiling the Potential a Novel Inorganic Perovskite for NTCThermistor and Multifunctional Application.

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## Abstract

The study synthesized a novel inorganic perovskite material, (Ni0.5Sm0.5FeO3)0.5(BaTiO3)0.5,exhibiting multifunctional characteristics, including potential multiferroic properties. Structural analysis revealed dual phase formation: 99.51% cubic phase (space group P m -3 m) and 0.49% cubic phase (space group F d -3 m). Using a scanning electron microscope (SEM), the morphology of the sample was examined. Using ImageJ software, the average grain size was calculated to be 461 nm. FTIR analysis identified key modes, while dielectric properties were evaluated across various frequencies and temperatures using an impedance analyzer. Room temperature dielectric studies indicate potential for storage applications. For NTC thermistor applications, the thermistor coefficient (β) and sensitivity factor (α) were evaluated by fitting data from the resistance variation with temperature graph.

## Introduction

The structural stability and functionality of materials are crucial for various applications. Perovskite-structured materials, known for their exceptional properties, typically meet these criteria with an ABX3 crystal structure. The unique ferroelectric and magnetic properties of ABO3 compounds stem from the d0 versus dn configuration issue. Recently, multiferroic (MF) materials have gained attention for their magneto-electric (ME) effect, useful in developing multifunctional devices like spintronics, sensors, and energy storage. Rare-earth ortho-ferrites (RFeO3) exhibit distorted perovskite structures with fascinating electrical and magnetic characteristics, making them potential candidates for next-generation storage devices and chemical sensors. SmFeO3 (SFO) is notable for its unique properties, including magnetization reversal, semiconducting properties, and significant piezoelectricity at room temperature. The magnetic properties of SFO are influenced by various interactions, making it suitable for spintronic and magnetoelastic devices. Research on BiFeO3 shows single-phase materials can exhibit both ferroelectricity and magnetism. Barium Titanate (BTO) is recognized for its outstanding ferroelectric and dielectric characteristics, making it an eco-friendly alternative to PZT. This study introduces Fe3+, Sm3+, and Ni3+ ions into the BaTiO3 lattice, resulting in a novel compound (Ni0.5Sm0.5FeO3)0.5(BaTiO3)0.5, thoroughly investigated for its structural, microstructural, dielectric, and magnetic properties to explore its multifunctional potential.

## Materials and synthesis technique

**1. Materials Used:** High-purity oxides and carbonates (99.99% purity, analytical reagent grade) from M/s Loba Chem. Pvt Ltd:
- BaCO3
- Sm2O3
- Ni2O3
- Fe2O3
- TiO2

**2. Weighing**: Exact amounts of these materials were weighed using a high-precision balance with accuracy up to three decimal places.

**3. Initial Grinding:**
- Ground thoroughly in dry air for 2 hours using an Agate mortar and pestle.

**4. Methanol Grinding:**
- Additional grinding with methanol until completely dry.

**5. Calcination:**
- The blended mixture was transferred to an alumina crucible.
- Calcined at 1200°C for 3 hours using a programmable high-temperature furnace.

**6. Crushing:**
- The calcined mass was crushed into fine, uniform powder using an Agate mortar and pestle.

**7. Pellet Formation:**
- Powder molded into pellets with polyvinyl alcohol (PVA) as a binding agent.
- Pellets compressed using a hydraulic pelletizing machine.

**8. Sintering:**
- Pellets sintered in a furnace at 1300°C for 4 hours to densify the material and remove any residual PVA.

## Set up

The Rigaku Ultima-IV X-ray diffractometer, using Cu-Kα radiation (λ=1.5406 Å), was employed to analyze phase formation and crystallinity in the synthesized compound over Bragg angles from 10° to 90° at a scanning rate of 2° per minute. A scanning electron microscope (Zeiss NTS Ltd. UK) was used to capture the topographic images of the powder sample, while purity was verified through EDX (EDX AMETEK) analysis. For the FTIR study, a Perkin Elmer SPECTRUM 100 and FRONTIER IR with a spectral range of 400-4000 $cm^{-1}$ (ATR mode) was used. Dielectric properties were investigated on the pellet specimen over frequency and temperature ranges of 100 Hz to 5 MHz and 300°C to 500°C, respectively, using a computer-controlled LCR meter (Model: PSM-1735). The leakage current of the samples was assessed using the I-V characterization method with a Keithley electrometer over a temperature range of 50°C to 500°C.

## Results

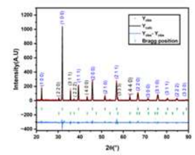

Fig1: Rietveld refinement using Full Prof software of the investigated sample.

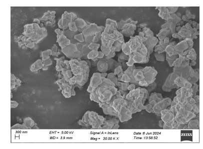

Fig2 : FESEM image of the investigated sample.

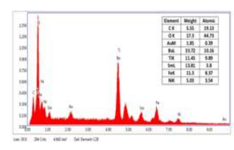

Fig3: EDX spectrum of the investigated sample.

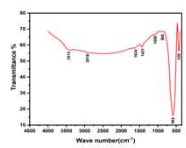

Fig4: FTIR spectra of the investigated sample.

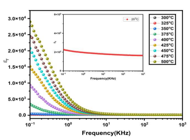

Fig5: Variation of εr with frequency at selected temperatures

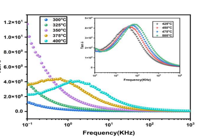

Fig 6: Variation of tanδ with frequency at selected temperatures

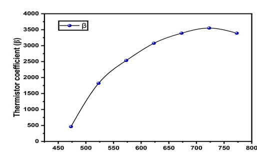


Fig7: thermistor constant ( β ) vs temperature.

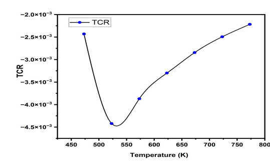


Fig8:Change in temperature coefficient of resistance( TCR ) with temperature

## Conclusions

This study investigates the novel material (Ni0.5 Sm0.5FeO3)0.5(BaTiO3)0.5, synthesized via the solid solution reaction method. It includes an analysis of structural, microstructural, elemental, dielectric, electric, and multiferroic properties. XRD analysis revealed two phases: 99.51% cubic (P m -3 m) with cell parameters a=b=c=8.339058 Å, α=β=γ=90°, and 0.49% cubic (F d -3 m) with a=b=c=3.964767 Å, α=β=γ=90°. SEM analysis showed a polycrystalline structure with grain formation and voids, with an average grain size of 461 nm. FTIR spectroscopy confirmed the perovskite phase. Dielectric spectra matched the Maxwell–Wagner model and suggested suitability for energy storage. I-V spectra indicated low leakage properties across temperatures. The material exhibited a high thermistor coefficient (β = 3549.43) and low sensitivity factor (α = -0.00679), making it suitable for NTC-thermistor applications.

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