Chapter 17 Study of the Solid Solution (Ba1-xSrx)2SmTi2Nb3O15 (x = 0-1)

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ABSTRACT

The compounds (Ba1-xSrx)2SmTi2Nb3O15 were synthesized via the solid-state method and characterized by X-ray diffraction (XRD) and impedance spectroscopy. The crystal structure is tetragonal, belonging to the P4bm space group. The lattice parameters (a = b, c, and V) decrease with increasing Sr substitution. Both the theoretical and experimental densities decrease as the Sr content rises. Impedance measurements show that all the compounds exhibit ferroelectric behavior, with the Curie temperature (Tc) decreasing from 332 °C (100% Sr) to 269.44 °C (100% Ba). Furthermore, impedance analysis allowed the determination of an equivalent electrical circuit. The AC conductivity spectra of the studied compounds follow Jonscher's power law. The relaxation process in the material is non-Debye type, and the temperature coefficient of resistance (NTCR) in the material is negative.

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INTRODUCTION

The family of tetragonal tungsten bronze (TTB) oxides exhibits interesting dielectric properties and is a potential candidate for various applications, such as electronic devices, sensors, and generators. Substitution at the pentagonal sites plays a crucial role in modifying the structure and electrical properties.

The general formula for tetragonal tungsten bronzes (TTBs) is written as follows: $(A_1)_2(A_2)_4(C)_4(B_1)_2(B_2)_8X_{30}$ (Gao et al., 2024; Løndal et al., 2024, 2025; Song et al., 2024; Tidey et al., 2024), where the A_1 and A_2 sites are occupied by alkali cations such as Na⁺, K⁺, or alkaline-earth cations like Ba²⁺ or Sr²⁺. The C site can be partially occupied by small cations such as Li⁺, Mg²⁺, or remain vacant, contributing to structural distortions. The B_1 and B_2 sites host transition metal cations such as Ti⁴⁺, Nb⁵⁺, or Ta⁵⁺. X_{30} represents oxygen or fluorine atoms that constitute the lattice.

TTBs oxides have a structure that is adaptable to cation substitutions. For instance, the insertion of Ba^{2+} cations into the A_1 sites increases the unit cell size and the dielectric constant (Neurgaonkar et al., 1988), while Sr^{2+} reduces lattice parameters but stabilizes the structural phases (Kolodiazhnyi et al., 2015). Substitution by Ti^{4+} , Nb^{5+} , or Ta^{5+} in the B_1 and B_2 sites influences both structural distortions and electrical properties (Chourti, Jalafi, et al., 2024). Lead-free TTB oxides offer an eco-friendly alternative with chemical stability and adaptable properties.

Lead-based ferroelectric compounds, such as lead titanate (PbTiO₃) and lead zirconate titanate (PZT), are widely used because of their excellent ferroelectric and piezoelectric properties, which arise from their well-defined perovskite crystalline structures. However, because of environmental concerns related to lead toxicity, intensive research is being conducted to develop lead-free ferroelectric materials. Among these, bismuth-based materials, such as $Na_{0.5}Bi_{0.5}TiO_3$ (NBT), and potassium-sodium niobate $K_{0.5}Na_{0.5}NbO_3$ or KNN, are particularly promising (JANOLIN, 2019; Zeb & Milne, 2013).

Lead-free materials like sodium-potassium niobate $(K_0.5Na_0.5)NbO_3$ or KNN, bismuth titanate $(Bi_4Ti_3O_{12})$, and barium titanate $(BaTiO_3)$ exhibit ferroelectric properties comparable to those of lead-based compounds but without their associated environmental drawbacks. For example, KNN-based ceramics have demonstrated high piezoelectric performance, making them suitable for various applications (Dolhen et al., 2015; JANOLIN, 2019).

The development of materials begins with a comprehensive understanding of the relationship between composition, structural properties, and ferroelectric characteristics, a topic that extensively studied by numerous researchers. For instance, lead-free materials such as $Sr_2(Sm_{1-x}Nd_x)Ti_2Nb_3O_{15}$ exhibit a progressive decrease in the Curie temperature, from 332 °C for x = 0 to 246 °C for x = 1. Additionally, the dielectric constant exceeds 127, while the dielectric loss ranges between 10^{-3} and 10^{-4} . Furthermore, lattice parameters increase with the substitution of Sm by Nd (Chourti et al., 2020). Materials such as $Sr_2GdTi_2Nb_3O_{15}$ exhibit thermal stability, a high dielectric constant, and low dielectric loss, making them promising for modern electronics applications (Chourti, Bendahhou, et al., 2024).

The global market is shifting toward the production of more sustainable and environmentally friendly materials. Future efforts should focus on optimizing dielectric properties, stabilizing ferroelectric phases at high temperatures, and integrating these materials into practical devices.

In this study, we will present the results of the substitution of alkaline-earth metals in the pentagonal (A2) sites of barium Ba^{2+} by strontium Sr^{2+} within the structure $(Ba_{1-x}Sr_x)_2SmTi_2Nb_3O_{15}$ (BSSTN, x = 0-1). Indeed, the BSSTN solid solutions are characterized using X-ray diffraction and dielectric measurements, with the aim of determining the structure and dielectric properties of these compounds. The objective is to correlate the composition, structure, and dielectric properties of the ceramics.

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