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Preparation and Piezo Properties of Potassium Sodium Tantalate system

Ragini Thapliyal[1] • Manish Uniyal*[1] • Surendra Singh[2]

[1]*Department of Physics,BGR Campus Pauri, H. N. B. Garhwal University, Uttarakhand*
[2] *Department of Sciences (Physics) Quantum University, Roorkee, Haridwar*

*Corresponding Author's Email Id: uniyaldrmanish@gmail.com

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Abstract: $Na_{1-x}K_xTaO_3$ (x = 0, 0.5) ceramics were synthesized via the solid-state route and sintered. XRD and SEM analyses confirmed an orthorhombic phase at room temperature, with refined lattice parameters and grain morphology. The piezoelectric response of $Na_{0.5}K_{0.5}TaO_3$ was further examined.

Key words: Ferroelectric ceramics • Piezoelectric materials • Crystallographic analysis • Surface morphology • P–E loop.

Introduction:

ABO_3-type tantalate perovskites represent a significant class of oxide materials exhibiting a wide spectrum of technologically important dielectric, piezoelectric, ferroelectric, and electro-optic properties (Bhatt et al., 2007). Sodium tantalate ($NaTaO_3$), belonging to the perovskite family, was first studied for its dielectric behavior by Matthias (1949), who reported a Curie temperature of 475 °C. Vousden (1951) subsequently determined, via room-temperature X-ray diffraction, that $NaTaO_3$ adopts an orthorhombic crystal structure characterized by lattice parameters a = 5.52 Å, b = 3.88 Å, and c = 5.47 Å. The compound retains an orthorhombic phase with space group Pbnm below 993 °C, transitioning to another orthorhombic phase with space group CmCm between 993 and 1126 °C. At 1108 °C, $NaTaO_3$ undergoes an additional phase transition to a tetragonal crystal structure with the space group P4/mmm. (Cross 1956; Iwasaki et al 1963; Kennedy et al 1999). At and above room temperature, $NaTaO_3$ exhibits antiferroelectric behavior with a Curie temperature of 475 °C. Recent advancements in piezoelectric and optoelectronic devices—such as high-speed electro-optic switches, modulators, and frequency doublers—have generated significant interest in perovskite tantalates as promising functional materials for next-generation technologies. Large, homogeneous single crystals are generally preferred for studying intrinsic material properties, as they reduce artifacts arising from surfaces and defects. However, single-crystal growth is often complex, time-intensive, and costly. In contrast, ceramics provide a simpler, more economical route to synthesis while retaining comparable functional performance (Bhatt et al 2007). Amorphous and nanocrystalline $NaTaO_3$ photocatalysts with porous structures have also been developed for overall water splitting (Tüysüz et al 2013). The microstructural characteristics of $(Na,K)NbO_3$ ceramics sintered under high alkaline vapor pressure were investigated by Acker et al (2014). López-Juárez et al. (2014) reported the rapid synthesis of $NaNbO_3$ and $Na_{0.5}K_{0.5}NbO_3$ using the microwave-assisted hydrothermal method (López-Juárez et al 2014). Kanhere et al (2013) explored the synthesis, photophysical properties, and photocatalytic performance of Bi-doped $NaTaO_3$ and Na_2TaO_3 nanoparticles. Theoretical and experimental studies on various ferroelectric ceramics have been conducted to clarify their fundamental characteristics (Uniyal et al 2011, 2012, 2014; Bhatt 2012). Scott (1989)

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reviewed the properties and potential of $Na_{1-x}K_xTaO_3$-based ferroelectric memories. There is growing interest in integrating ferroelectric thin films into optoelectronic integrated circuits (Wessels 1998). In ferroelectric materials, birefringence can be induced by static or alternating electric fields. Effective integration of ferroelectric layers into optoelectronic devices demands fulfillment of specific material criteria (Wessels 2004). Previously, our group has investigated the structural, dielectric, and piezoelectric properties of sodium–potassium niobate and lead magnesium niobate, as well as the ultrasonic and electrical behavior of ferrofluids (Uniyal et al 2003, 2015, 2018, 2019; Singh et al 2001; Singh et al 2018; Kashyap et al 2020a, 2020b; Saxena et al 2020). This study aims to synthesize, characterize, and evaluate the piezoelectric properties of $Na_{0.5}K_{0.5}TaO_3$, thereby providing a reliable reference for selecting appropriate materials in targeted device applications. These ceramics show promise for second harmonic generation, delay line devices, and other optoelectronic technologies.

Experimental Procedure:

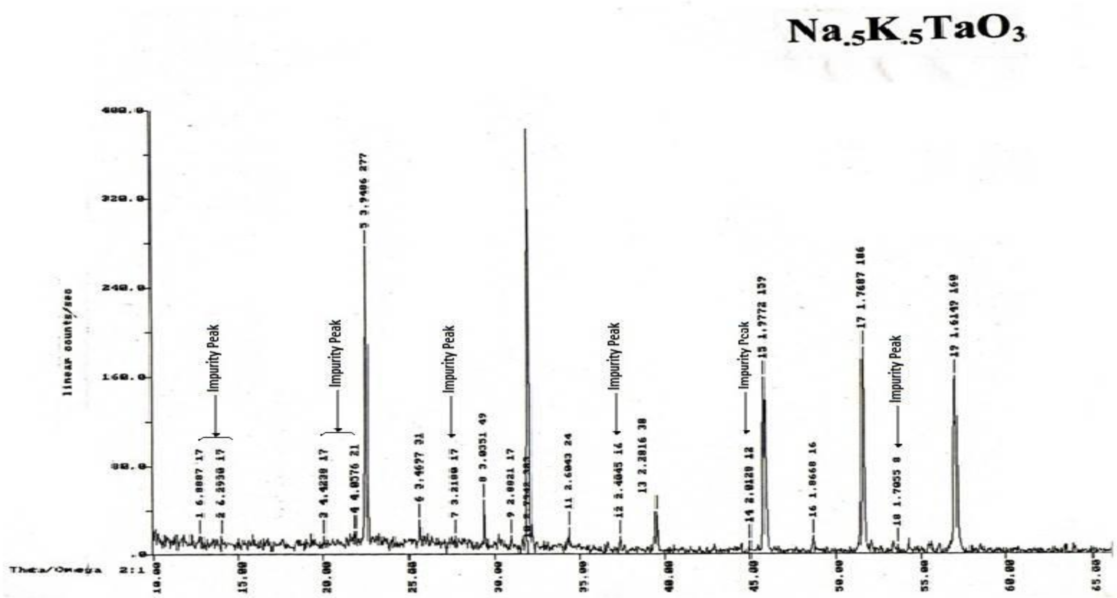

Fig 1: X-ray diffraction pattern of $Na_{0.5}K_{0.5}TaO_3$

$Na_{0.5}K_{0.5}TaO_3$ was synthesized using sodium carbonate, potassium carbonate (Qualigens Fine Chemicals), and tantalum pentoxide (99.9%, FlukaChemie AG). Precursors were dried at 200 °C for 1 h, mixed in stoichiometric ratios, and calcined in air at 950 °C for 2 h in a platinum crucible to ensure complete carbonate decomposition. The calcined powder was cooled, reweighed, reground, and uniaxially pressed into 10 mm pellets, then sintered at 1050 °C for 26 h in air.

Characterization:

X-Ray Diffraction (XRD):

Room-temperature XRD patterns were recorded using a SEIFERT (Bruker) diffractometer with Cu-Kα radiation (λ = 1.540598 Å), calibrated using a silicon standard. Peaks were indexed with the JCPDS database, and lattice parameters were derived from 2θ data. Unit cell refinement was performed using Auto-X software with CRYSFIRE and FULLPROF integration.

The XRD patterns of the prepared samples revealed characteristic reflections corresponding to both orthorhombic and cubic perovskite phases, accompanied by minor impurity peaks, as illustrated in Fig. 1. Impurity peaks in the $Na_{0.5}K_{0.5}TaO_3$ ceramic are explicitly labeled. Refined lattice parameters for all compositions are compiled in Table 1.

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Table -1: Variation in lattice parameters occurs when potassium (K) is substituted for sodium (Na) in $NaTaO_3$.

Composition	Lattice parameters		
	a(Å)	b(Å)	c(Å)
$Na_{0.5}K_{0.5}TaO_3$	5.588	5.581	5.585

Scanning Electron Micrographs (SEM): Surface morphology was analyzed using a LEO 440 scanning electron microscope (SEM). SEM micrographs of the $Na_{1-x}K_xTaO_3$ samples are shown in Fig. 2, and the corresponding grain size estimates are listed in Table 2.

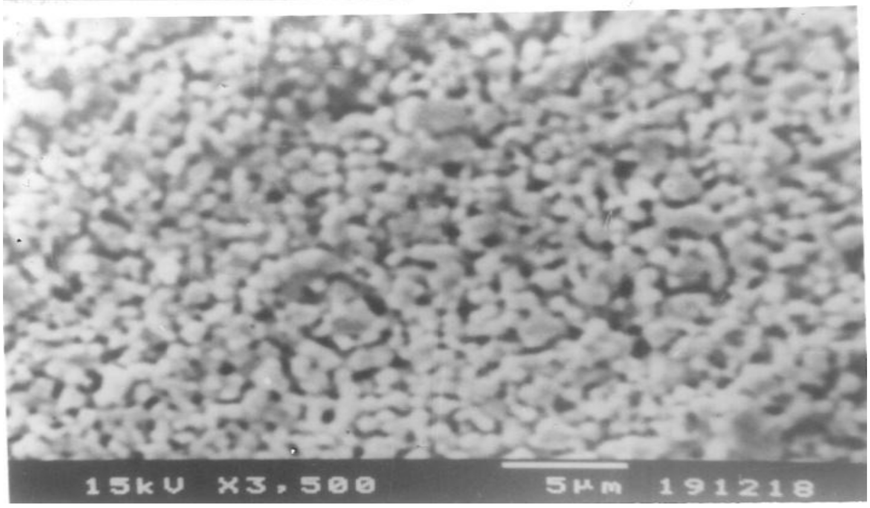

Fig.2. Scanning Electron micrographof $Na_{0.5}K_{0.5}TaO_3$

Table–2: Grain Sizes for $Na_{0.5}K_{0.5}TaO_3$.

Composition	Grain Size (μm)
(Na,K)TaO_3	6.87

Piezo Properties

For piezoelectric evaluation, sintered $Na_{0.5}K_{0.5}TaO_3$ pellets were electroded with air-dryable silver paste in a parallel-plate (metal–insulator–metal, MIM) configuration and tested under an applied field of 100 V. The polarization–electric field (P–E) hysteresis loops and piezoelectric coefficients were measured using a ferroelectric loop tracer and a piezoelectric evaluation system (AixACCT Systems GmbH).

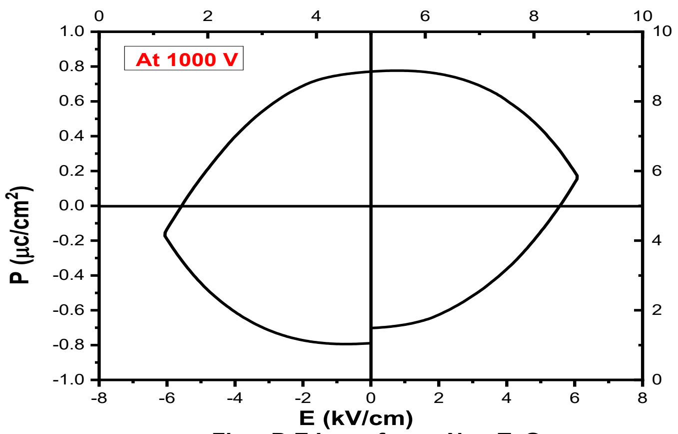

Fig. P-E Loop for $_{K0.5}Na_{0.5}TaO_3$

Result and Discussion:

X-ray diffraction (XRD) patterns of the synthesized samples reveal characteristic peaks corresponding to a cubic perovskite structure, with minor impurity phases, as depicted in Fig. 1. Structural analysis confirms the cubic phase, in agreement with prior reports (Murthy, 1990). Refined lattice parameters for all compositions are presented in Table 1, supporting the assigned crystal symmetry.

Scanning electron microscopy (SEM) micrographs of the $Na_{1-x}K_xTaO_3$ ceramics are shown in Fig. 2, highlighting their microstructural characteristics. Polarization–electric field (P–E) hysteresis loops for unpoled $Na_{0.5}K_{0.5}TaO_3$ samples, recorded at room temperature under an applied field of 1000 kV/cm, are displayed in Fig. 3. The well-saturated loops confirm the ferroelectric nature of the material. The observed high remnant polarization and converse piezoelectric coefficients at low applied fields are comparable to those of modified PST ceramics, underscoring their suitability for device applications.

Conclusion:

Substitution of K^+ for Na^+ in $NaTaO_3$ results in a systematic increase in lattice parameters, consistent with the larger ionic radius of K^+ and the associated lattice distortion. SEM analysis indicates that average grain size increases with rising potassium content, reflecting enhanced grain growth during sintering. The P–E hysteresis loops of all $Na_{1-x}K_xTaO_3$ compositions display well-saturated behavior, confirming their ferroelectric character.

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