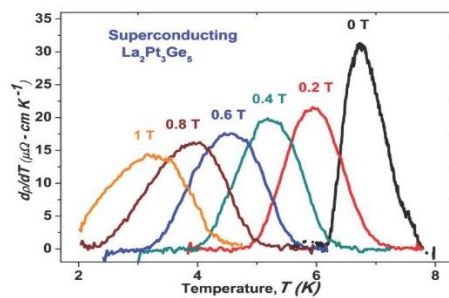


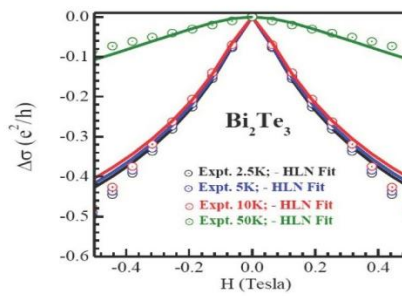
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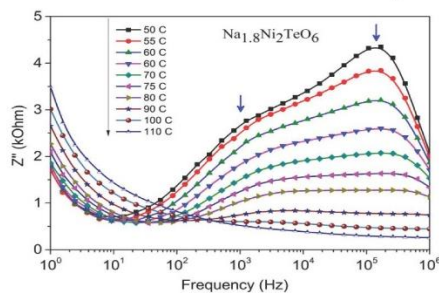
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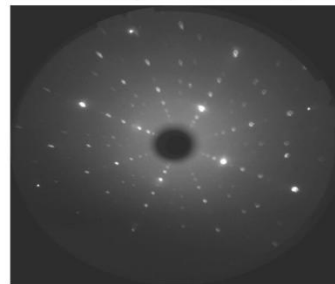
First order derivative of resistivity



Magneto-conductivity



Imaginary part of impedance (Z'')



Laue diffraction pattern of SnTe(100)

Important influence of Bi deficiency on the conducting property of $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ perovskite oxide

B. Santhoshkumar; P. Lokeswara Rao; K. V. Ramanathan; A. K. Bera; Bholanath Pahari 

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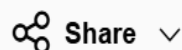
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Recently it has been reported that low levels of Bi nonstoichiometry (only ± 1 atomic %) in the nominal starting composition of $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ (NBT) ceramics can lead to dramatic changes in the conduction property. Present article present the results of powder XRD,

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Anil Arya; Mohd Sadiq; A. L. Sharma

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B. Santhoshkumar; P. Lokeshwara Rao; K. V. Ramanathan; A. K. Bera; Bholanath Pahari

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Important Influence of Bi Deficiency on the Conducting Property of $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ Perovskite Oxide

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Abstract. Recently it has been reported that low levels of Bi nonstoichiometry (only ± 1 atomic %) in the nominal starting composition of $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ (NBT) ceramics can lead to dramatic changes in the conduction property. Present article present the results of powder XRD, ^{23}Na MAS NMR and impedance spectroscopy in nominal starting compositions, $\text{Na}_{0.5}\text{Bi}_{0.5+x}\text{TiO}_{3+3x/2}$ with $x = 0.0$ and -0.02 . Room temperature XRD data analysis indicates both NBTs have a rhombohedral (space group $R3c$) structure. While, ^{23}Na MAS NMR results demonstrate a complex local structure and significant disordering of Na coordination environment. Impedance spectroscopy reveals high levels of oxide-ion conduction in NBT. 2 at-% Bi-deficient NBT ($\text{Na}_{0.5}\text{Bi}_{0.48}\text{TiO}_{2.97}$) exhibits higher conductivity of $\sigma \sim 1.3 \times 10^{-4}$ S/cm at 500 °C and activation energy, $E_a = 0.85$ eV. Present results therefore substantiate the A-site nonstoichiometry sensitive electrical property of NBT.

1. INTRODUCTION

The perovskite oxide $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ based solid solution material is one of the extensively studied piezoelectric material. It replaces well-known lead zirconate titanate [$\text{Pb}(\text{Zr}_{1-x}\text{Ti}_x)\text{O}_3$, PZT] for applications in actuators, sensors, and transducers [1]. There is a considerable amount of controversy on the room temperature crystal structure of NBT. A rhombohedral structure ($R3c$) was confirmed by neutron diffraction studies [2]. Later high resolution synchrotron powder X-ray diffraction data proposed a monoclinic structure with space group Cc [3]. In addition to that it is observed that the average structure determined by neutron and x-ray diffraction is different from the complex local structure studied by extended x-ray absorption fine structure (EXAFS) analysis [4]. The complex nature of the local structure has profound impact on the perceived global structure and ferroelectric properties. Results of transmission electron microscopy (TEM), pair distribution function (PDF) analysis are also recently reported by different groups. But true structure is not understood yet.

Interest in NBT has expanded recently soon after the discovery of dramatic influence of A-site nonstoichiometry on the conduction property by Li *et al.* The reported NBT with general formula $\text{Na}_{0.5}\text{Bi}_{0.5+x}\text{TiO}_{3+3x/2}$ is an oxygen-ion conductor for $x = 0.0$ (NBT). Significantly higher oxygen-ion conductivity $\sim 10^{-3}$ S cm^{-1} at 500 °C is measured for $x = -0.01$ ($\text{NB}_{0.49}\text{T}$) composition. Bi excess composition with $x = 0.01$ ($\text{NB}_{0.51}\text{T}$) whereas is an insulator [5]. High oxygen ion conductivity in NBT and $\text{NB}_{0.49}\text{T}$ is attributed to the high oxide-ion mobility associated weak Bi-O bonds. This report has opened a new application possibility of NBTs as electrolyte material for intermediate temperature solid oxide fuel cells (ITSOFC) because total conductivity of $\text{NB}_{0.49}\text{T}$ is higher than the well-known SOFC electrolyte, yttria-stabilized zirconia (YSZ) [6]. Therefore, it is also important to understand how such a small compositional change in the A-site stoichiometry of the undoped perovskite can induce high levels of oxygen-ion conductivity. In this article, we present the results of powder XRD, ^{23}Na MAS NMR and impedance spectroscopy