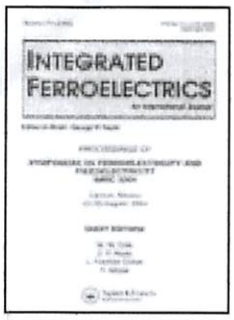

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Effects of calcination temperature on the synthesis of $[KNbO_3]_{0.9} - [BaNi_{0.5}Nb_{0.5}O_3]_{0.1}$ perovskite powders

Saichon Sriphan[a,b], Suwit Kiravittaya[a,b,c], and Theerachai Bongkarn[b,c,d]

[a]Advanced Optical Technology (AOT) Laboratory, Department of Electrical and Computer Engineering, Faculty of Engineering, Naresuan University, Phitsanulok, Thailand; [b]Research Center for Academic Excellence in Applied Physics, Faculty of Science, Naresuan University, Phitsanulok, Thailand; [c]Research Center for Academic Excellence in the Petroleum, Petrochemicals and Advanced Materials, Naresuan University, Phitsanulok, Thailand; [d]Department of Physics, Faculty of Science, Naresuan University, Phitsanulok, Thailand

ABSTRACT

The phase and structural properties of $[KNbO_3]_{1-x}$ - $[BaNi_{0.5}Nb_{0.5}O_3]_x$ (KBNNO) perovskite powders with $x = 0.1$, which have been prepared by using the combustion technique, are reported. The investigated calcination temperatures are between 500°C and 1000°C. The perovskite structure phase is found for all samples. All main peaks in X-ray diffraction (XRD) patterns can be correlated with $KNbO_3$ cubic structure (JCPDS no. 08-0212). Highly pure perovskite crystalline phase is found in the sample calcined at 650°C, which is about 100 – 250°C lower than that of the conventional solid-state reaction technique. However, the impurity phases occur in the samples calcined in temperature range between 700°C and 1000°C. These impurity phases might originate from contamination of atmospheric oxygen or other matters. By continuously varying dwell time, we found a suitable condition for synthesis KBNNO powder, which is the calcination temperature of 650°C and the dwell time of 1.5 h. This result is confirmed by the calculated percent perovskite, XRD peak intensity and width. The crystalline size calculated by using Scherrer's equation, which is around 21 – 24 nm, tends to increase with the increase of calcination temperature and dwell time. Rietveld refinement method is applied to determine the lattice parameters of both tetragonal $KNbO_3$ and hexagonal $BaNi_{0.5}Nb_{0.5}O_3$.

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1. Introduction

Ferroelectric (FE) materials are one of the materials which have a spontaneous polarization occurred below the transition temperature and their polarization direction can be reversed using an external electric field [1]. These materials have been proposed for replacing conventional materials in electronic device applications

CONTACT Suwit Kiravittaya Suwitki@gmail.com
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such as dielectric material in capacitor [2], random-access memory [3], actuator [4], and sensor [5] as well as photo-absorber in photovoltaic (PV) cells [6–10]. PV mechanism in FE materials is different from conventional semiconductor devices, which need built-in electric field for extracting photogenerated carriers. In ferroelectric photovoltaic (FE-PV) cell, the photoelectrons and holes can be separated by the spontaneous polarization occurred from asymmetry structure [11]. The interesting phenomena in FE-PV are fundamentally different from a conventional PV cell in many aspects. For examples, (1) the output photo voltage will not be limited by material band gap [12] and (2) the direction of the output photo current can be changed by tuning the polarization direction of FE material [11,13].

Generally, FE-PV cells, which are fabricated by the standard FE ceramics such as barium titanate or lead zirconate titanate, have very low conversion efficiency [14–16]. This is due to their wide band gap ($E_g > 3$ eV) and therefore the extracted photoelectrons have insufficient energy for exciting to the conduction band. Nowadays, researchers are investigating the PV effect in many FE materials. One of the most investigated FE-PV materials is $BiFeO_3$. It provides a conversion efficiency (η) better than other materials. A short-circuit current density (J_{sc}) in the range of $\mu A/cm^2$ to mA/cm^2, an open-circuit voltage (V_{oc}) of 0.50 – 0.60 V and η of $\sim$ 0.06% can be found in this material because of its low band gap ($E_g \sim 2.7$ eV) [9–10]. This material absorbs 20% of the solar spectrum. For more absorbing photon in visible light region, researchers thus try to design other FE-PV materials that provide a lower E_g. Choi et al. [7] have reported that the doping of $LaCoO_3$ into $Bi_4Ti_3O_{12}$ thin film can reduce E_g of $Bi_4Ti_3O_{12}$ from 3.55 to 2.65 eV. Moreover, non-perovskite $KBiFe_2O_5$ material, which has been developed by Zhang et al. [8], can also reduce E_g to 1.60 eV. However, the obtained E_g from these materials does not cover visible light region yet. Recently, the first visible light absorbing perovskite $[KNbO_3]_{1-x}$ - $[BaNi_{0.5}Nb_{0.5}O_{3-\delta}]_x$ (KBNNO) has recently been discovered by Grinberg et al. [6]. This material is very interesting for using in PV application because it can absorb more photon in visible light range. At $x = 0.1$, they reported that KBNNO has the highest polarization values, which are saturation polarization (P_s) $\sim 20\ \mu C/cm^2$ and remnant polarization (P_r) $\sim 5\ \mu C/cm^2$, with $E_g \sim 1.4$ eV. The reported PV performance of their work is still quite low (J_{sc} is 40 nA/cm^2 and V_{oc} is 3.50 V for 500-V poled KBNNO with $x = 0.1$). This might be due to the lack of some optimization steps in the fabrication process. In this work, the $[KNbO_3]_{1-x}$ - $[BaNi_{0.5}Nb_{0.5}O_3]_x$ powders with $x = 0.1$ are prepared by using a solid-state combustion technique. In this method, a reaction-speed up energy provided by fuel material is generated. It can reduce the heating temperature and dwell time while keeping high quality powders/ceramics [19–20]. The powder preparation conditions are investigated. The effects of calcination temperature and dwell time on the obtained structural phases and microstructure of KBNNO with $x = 0.1$ are discussed.