Optik 158 (2018) 199–203

Contents lists available at ScienceDirect

Optik

journal homepage: www.elsevier.de/ijleo

Original research article

Effect of the synthesis conditions on the structural, morphological and optical properties of $Bi_2Te_{2.7}Se_{0.3}$ nanoparticles

H.M. Ali, E.M.M. Ibrahim*, M.M. Wakkad, M.A.A. Mohamed

Physics Department, Faculty of Science, Sohag University, Sohag 82524, Egypt

ARTICLE INFO

Article history:
Received 12 November 2017
Accepted 19 December 2017

Keywords:
Bi_2Te_3
Physical vapour deposition
Optical
Chalcogenide
Kubelka-Munk theory

ABSTRACT

Beside their promising utility as thermoelectric generators, Bi_2Te_3 and related compounds have several applications in electronic and optoelectronic devices. In this work, $Bi_2Te_{2.7}Se_{0.3}$ nanoparticles (NPs) were successfully prepared via physical vapor deposition technique at different conditions of flow rate and temperature. The x-ray diffraction patterns show that, the NPs crystallize in a rhombohedral crystal structure with preferable growth along the (015) plane. Field-emission scanning electron microscope (FE-SEM) investigation shows that the NPs size depends significantly on the synthesis conditions of flow rate and temperature where it decreases with the decrease in the former or with the increase in the later. The effect of deposition conditions on the final morphology can be interpreted through the accompanied variation in the concentration of the gaseous precursors in the hot zone. The optical properties were studied using Kubelka-Munk theory. Optical band gaps of 0.52, 0.58, 0.53 eV were determined for the samples synthesized under different conditions.

1. Introduction

Bi_2Te_3 and its based solid solutions are layered structure with rhombohedral unit cell (space group:R-3m) such that the bismuth and tellurium atoms are arranged in parallel layers following the sequence $Te^{(1)}$-Bi-$Te^{(2)}$–Bi-Te [1] which is continually repeated [1]. In addition to their efficiency as thermoelectric materials [2–5] which culminated in the fabrication of thermoelectric generator and thermo-coolers, these compounds have several applications in electronics, microelectronics, optoelectronics and electromechanical devices [6]. For example, such compounds are used as photoconductive targets in TV cameras, IR spectroscopy, IR detectors and sensors [7–10]. Also, Bi_2Te_3 is a narrow band gap semiconductor and thus it could be exploited in other applications like temperature controller in laser diode [11] and optical recording system [12]. According to the presence of point defects, Bi_2Te_3 can exhibit either p- or n- type conduction but n-type is the most common as a result of considerable amount of anti-site point defects through the occupying of Te site with bismuth site [6].There are several strategies that were introduced to improve the thermoelectric performance of Bi_2Te_3 like doping, nanostructuring and nanocomposites [13].

Indeed, a great enhancement was achieved especially in nanostructures which can be attributed to the increase of density of states (DOS) and the decrease in the thermal conductivity through the scattering of the phonons across the boundaries [14]. Doping with antimony (Sb) [15] and selenium (Se) [16] is adopted strategy in order to enhance the physical properties of

* Corresponding author.
E-mail address: e.ibrahim@science.sohag.edu.eg (E.M.M. Ibrahim).

https://doi.org/10.1016/j.ijleo.2017.12.090
0030-4026/

Table 1
XRD parameters of the synthesized samples.

Sample	FWHM	D_{XRD}(nm)	ρ $(nm)^{-2}$ $(10)^{-3}$	ε $(10)^{-3}$
(A)	0.478	17.22	3.3	2
(B)	0.299	27.48	1.3	1.2
(C)	0.276	29.77	1.1	1.1

Bi_2Te_3. There are various techniques that are used for the synthesis of Bi_2Te_3 based compounds such as thermal evaporation [17], co-sputtering [18] molecular beam epitaxy [19], solvothermal method [20],etc. In this work, $Bi_2Te_{2.7}Se_{0.3}$ compound has been synthesized by physical vapor deposition (PVD) method. Although, this compound has fuelled an intense research as an efficient thermoelectric material, few papers that focused on studying the effect of deposition on its structure, morphology and optical properties which have been presented here.

2. Experimental method

$Bi_2Te_{2.7}Se_{0.3}$ NPs were synthesized from a bulk alloy as a source material using the physical vapor deposition (PVD) technique and the procedures can be summarized as the following: (i) The source material was placed in the hot zone at a certain temperature (T) to transform the solidus material to gaseous phase. (ii) Argon gas (Ar) was used as a carrier gas to transport the NPs formed in the gaseous phase to the cold zone. (iii) The $Bi_2Te_{2.7}Se_{0.3}$ NPs were deposited on glass substrates placed in the cold zone at temperature not higher than 200 °C. (iv) After furnace cooling to the room temperature, the deposited NPs were extracted from the cold zone for carrying out the various investigations and measurements.

Noteworthy, three samples of deposited $Bi_2Te_{2.7}Se_{0.3}$ NPs were synthesized at different conditions of temperature and flow rate, specifically, (1035 °C, 270 SCCM), (825 °C, 270 SCCM) and (825 °C, 225 SCCM) and denoted in the following as sample A–C, respectively as a matter of facilitation. The samples were characterized using the x-ray diffraction (XRD) (Brucker Axs-D8 Advance diffractometer with Cu-K_α radiation at $\lambda = 0.154178$ nm). The surface morphology and structure were demonstrated using scanning electron microscope (SEM) model: Quanta FEG250 for imaging the surface morphology. To study the optical properties of the synthesized samples, A Jascov-570 UV–vis-NIR spectrophotometer was employed to record the reflection spectrum over the wavelength range 200–2500 nm at both normal incidence and room temperature. Diffuse reflectance spectrum was obtained using a diffuse reflectance accessory model ISN-470, and the reflectance was converted by the instrument software to F(R) values according to Kubelka-Munk method.

3. Results and discussion

3.1. Structure and morphology

3.1.1. Effect of deposition conditions on the structure

Fig. 2a shows the XRD pattern of the synthesized samples A–C. The data confirm that the NPs for all samples crystallize in polycrystalline rhombohedral structure with preferential orientation along (015) direction. With respect to the sample (A), all peaks can be indexed to Bi_2Te_3 compound with preferable growth through (015) plane. The peaks can be indexed using standard reflection data of JCPDS card no. 85–0439. The sharpness of the peaks confirms the good crystallinity of the products. No additional peaks correspond to Te, Se, Bi or other impurities were observed indicating to the high purity of the sample.

The x-ray pattern of sample (B) reveals that the phase is Te-rich Bi_2Te_3 indicating the simultaneous co-existence of Bi_2Te_3 and Te atoms (denoted by *). Additional small peak corresponding to Bi (denoted by ♦) could be observed. Noteworthy, the strong appearance of Te peaks here can be attributed to the decrease in temperature in the hot zone. Where, once the thermal decomposition of the bulk alloy occurs, the elements begin to evaporate with different evaporation rate [21]. The decrease in temperature with fixing the flow rate of argon leads to a reduce in the concentration of the gaseous precursors in the hot zone and hence, the chance of Bi atom to meat and react with Te atom in the hot zone decreases which make limitation for the growth of Bi_2Te_3 phase. This hypothesis is also assured if we take in consideration that the nucleation and growth of Te atoms is faster than Bi_2Te_3 [22].

The x-ray data of sample (C) illustrates a decrease in the intensity of the Bi and Te peaks as shown in Fig. 2a. The reason for the lack of Te and Bi phases here can be attributed to the increase of the concentration of gaseous precursors in the hot zone compared to sample (B) due to the decrease in the flow rate which leads to the increase of the chance of Bi and Te atoms to react and form Bi_2Te_3 compound.

The average crystallite size (D_{XRD}) was calculated using Debye–Sherrer's equation [23] $D = 0.9\lambda/\beta \cos\theta$ where, θ is the glancing angle, λ is the wavelength of Cu k_α radiation ($\lambda = 1.5406$ Å) and β is the full width at half maximum. Also, The dislocation density(ρ) which assess the proportion of defects through the samples is calculated using this formula $\rho = 1/(D_{XRD})^2$ [24]. It is well known that as the crystallite size becomes smaller the lattice strain (ε) becomes larger and the x-ray diffraction peak becomes broader [25]. The strain is calculated using this formula $\varepsilon = \beta \cos\theta/4$ [26]. All the previously mentioned x-ray parameters are tabulated in Table 1.