

Structural Properties of $Zn_xBi_{2-x}Te_3$ alloys prepared by solid solution

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ABSTRACT

In this research study ($Zn_xBi_{2-x}Te_3$) ternary alloys are prepared using solid solution by varying the Zn elements amount (x) from (0- 0.3). Samples were prepared in a furnace at (700 °C) for (6 h) to enhance homogenous distribution in alloys. Alloys were characterized by (XRD). Results showed that the Bi_2Te_3 and its alloys were a polycrystalline and having high direction at (015) plane in $2\theta = 27.37$ degree while the alloys at (0015) in $2\theta = 45.12$ degree and the intensity of the peak increase by increasing Zn amount except in $x=0.2$. A shift in planes presence due to creation of (ZnTe) compound and increase in grain size.

Keywords:- Bismuth Telluride, Ternary alloys, $ZnBiTe$, XRD,

1. INTRODUCTION

Bi_2Te_3 is a gray powder of Bismuth and Tellurium also known as Bismuth (III) Telluride. It is a semiconductor which, when alloyed with Antimony or Selenium become an efficient thermoelectric material for refrigeration or portable power generation [1]. Topologically protected surface states have been observed in Bismuth Telluride [1]. Bi_2Te_3 compounds as well as some related ternary alloys are often used for cooling applications in commercial Peltier elements. Commonly applied ternary alloys consist of Bismuth Telluride with either Bismuth Solenoid (Bi_2Se_3) or antimony Telluride (Sb_2Te_3) [2]. The crystal structure of Bismuth Telluride is rhombohedral as shown in Figure (1) with hexagonal unit cell [3], [4]. Whereas the hexagonal description outlines the layered structure of the material, its unit cell has lattice constants ($a = 4.38 \text{ \AA}$) and ($c = 30.36 \text{ \AA}$) at 77° K [5]. The structure can be visualized as Bi and Te layers stacked along the c -axis in the unit cell with van der Waals bonding between the layers [6], [7]. The non-cubic structure of bismuth telluride contributes to anisotropy in thermoelectric properties, to physical characteristics (easy cleavage along the basal plane), as well as to the diffusion coefficients of impurities or dopants [8], [9]. Its structure with space group $R3m$ and the lattice are stacked in a repeated sequence of five atom layers: $Te_1-Bi-Te_2-Bi-Te_1$ along the c -axis (Figure 1). The superscripts 1 and 2 denote differently bonded tellurium atoms. Te and Bi layers are held together by strong ionic-covalent bonds (Te_1-Bi and $Bi-Te_2$). The Te_1 bonds between cells are of the van der Waals type and are extremely weak.

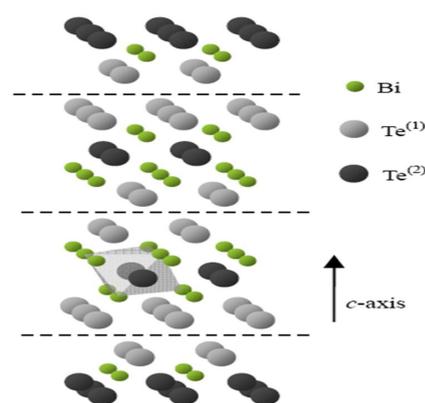


Figure (1) the crystal structure of Bi_2Te_3 [9].

The preferential orientation of XRD spectrum of Bi_2Te_3 is (015) plane at ($2\theta = 27.6^\circ$) [9], [14]-[18]. Adding impurities tend to cause a new pre dominant plane, where adding Cr enhanced the (110) and cause a new orientation (0015) planes, while using Se increase the intensity of the (0018) plane [19],[21]. There are eight fields of primary crystallization on the liquids surface of the Zn-Bi-Te ternary system (figure 1.5) [22]. The field of ZnTe crystallization lodges almost all liquids surface. Two immiscibility regions exist in this system. One of them adjoins to the Zn-Bi binary system and forms narrow band in the Zn- Bi- Te ternary system, and the other is located inside the triangle along the ZnTe- Bi quasibinary system. Nonvariant equilibria in this ternary system are given in table 1

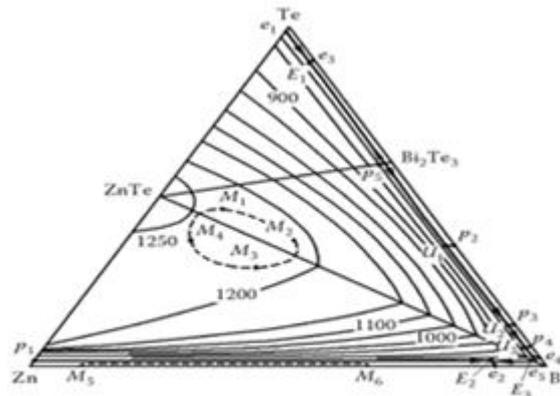


Figure (5) primary crystallization on the liquids surface of the Zn-Bi- Te ternary system

Table 1 The Nonvariant equilibria in ternary system

symbol	Reaction	T, °C
P ₅	$L + ZnTe \leftrightarrow Bi_2Te_3$	600
E ₁	$L \leftrightarrow ZnTe + Te + Bi_2Te_3$	410
E ₂	$L \leftrightarrow ZnTe + Zn + Bi$	250
E ₃	$L \leftrightarrow Bi_{14}Te_3 + Bi + ZnTe$	260
U ₁	$L + Bi_2Te_3 \leftrightarrow ZnTe + BiTe$	545
U ₂	$L + BiTe \leftrightarrow ZnTe + Bi_2Te_3$	415
U ₃	$L + Bi_2Te_3 \leftrightarrow ZnTe + Bi_{14}Te_6$	310

2. PROCEDURE

Bi₂Te₃ and Zn_xBi_{2-x}Te₃ targets were prepared in this work by take the ratio (2:3) of atomic weight for Bismuth (99.999%) to Tellurium (99.99%) with small portions of Zinc (99.999%) all materials were purchase from Aldrich. By charging a mixing of an accurate amount of Zinc, Bismuth and Tellurium powder in an evocated quartz tube then putted in a furnace at (700 °C) for (6 h) to enhance homogenous distribution in alloys. All other targets Zn_{0.1}Bi_{1.9}Te₃, Zn_{0.2}Bi_{1.8}Te₃, Zn_{0.3}Bi_{1.7}Te₃, are alloying by the same way.

3.RESULTS

To evaluate the crystalline and the orientation of alloys, X- ray diffraction was used for this purpose. The results of X- ray diffraction of material prepared in this work, p-Bi₂Te₃, p-Zn_{0.1}Bi_{1.9}Te₃, p-Zn_{0.2}Bi_{1.8} Te₃ and Zn_{0.3}Bi_{1.7}Te₃ are shown in figures (2), (3), (4) and (5) respectively of all these four alloys. The (XRD) pattern for pure Bi₂Te₃ as shown in figure (2) , a strong preferential orientation at (2θ =27.79)° of [015] plane with minor peaks corresponding to value of (2θ) at(21.74°,38.28°,40.8°,62.8° and 72.3°) for[101], [1010],[110],[0210] and [2110] respectively in comparable with ASTM card Bi₂Te₃. The diffracted peaks indicated that the target is polycrystalline with hexagonal unit cell according to the powder diffraction file for PC (PCPDF) (08-(027) with space group R3m having (a=0.43 nm, c=2.99 nm) whereas the [015] diffraction peak is expected to be the most intense for randomly oriented polycrystalline Bi₂Te₃ samples for this card. Figures (3), (4) and (5) show a change in the strongest preferential orientation at (2θ =44.27)°, (2θ =44.75)° and (2θ =44.74)° respectively of [0015] as the addition of Zn element. These orientation intensities are varying according to the variation in Zn amount. The position of the diffraction lines have small shift in the peak position relative to [ZnTe] peaks. This indicates that there is a change in target composition from the ideal Bi:Te stoichiometry of 2:3 alloy to ZnTe/Bi₂Te₃ alloy moreover, those targets present a less strong <015> orientation. ZnTe peaks are shown at (2θ =41.54)°, (2θ =57.13)° and (2θ =64.25)° for (110), (202) and (203) planes respectively. A summary of the data obtained from targets is given in table (2) .It was clearly recognized that sample C having different behavior by increasing Zn to decrease [0015] peak intensity, where sample B and D have peak intensity greater than C i.e. in Zn_{0.2}Bi_{1.8}Te₃ tend to having properties as same as the pure material. The corresponding lattice parameters are a =53 nm, b = 53 nm, and c = 33.36 nm.

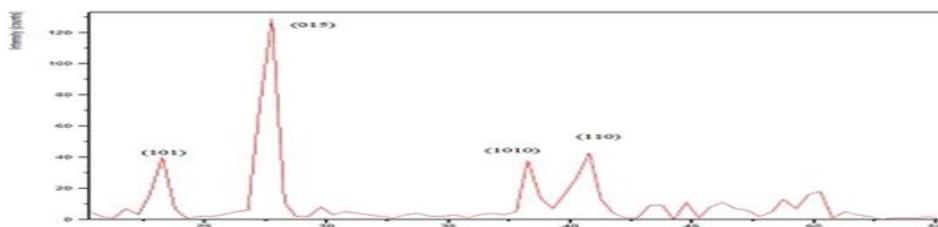


Figure (6): X-ray diffraction pattern of p-Bi₂Te₃ alloy.

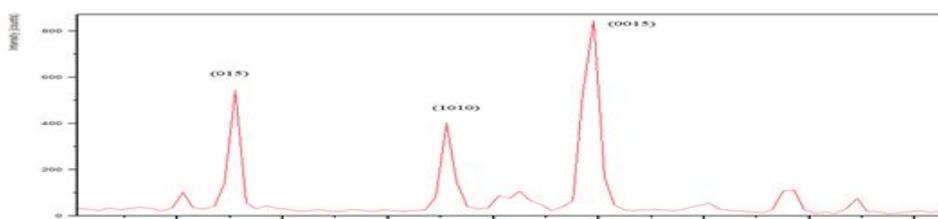


Figure (7): X-ray diffraction pattern of Zn_{0.1}Bi_{1.9}Te₃ alloy

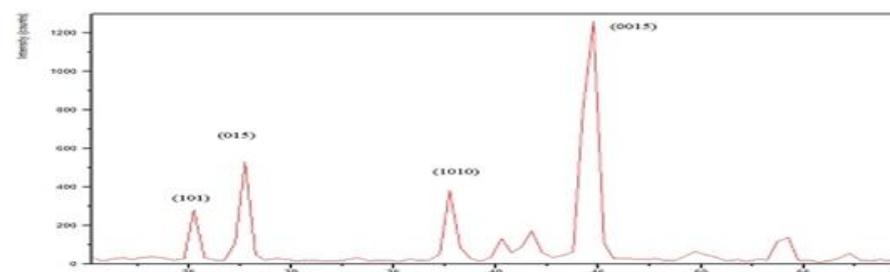


Figure (8): X-ray diffraction pattern of targets p- Zn_{0.2}Bi_{1.8}Te₃ alloy

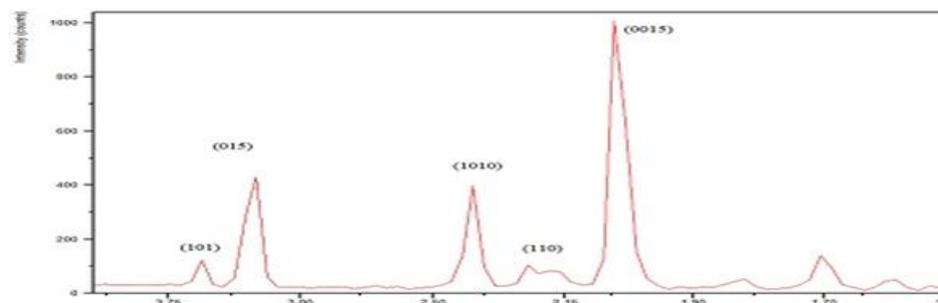


Figure (9): X-ray diffraction pattern of targets p-Zn_{0.3}Bi_{1.7}Te₃ alloy

Table (2) Summary of the data obtained from targets

Material	2θ degree ASTM	2θ degree Exp.	D (Å) ASTM	D (Å) Exp.	Intensity (a.u)	Δ 2θ degree	hkl
Bi ₂ Te ₃	27.616	27.79	3.23	3.37	129	-0.14	(015)
	45.439	44.78	1.996	2.05	10	-0.054	(0015)
Zn _{0.1} Bi _{1.9} Te ₃	27.616	27.78	3.23	3.207	428	-0.164	(015)
	45.439	44.72	1.996	2.04	1004	0.719	(0015)
Zn _{0.2} Bi _{1.8} Te ₃	27.616	27.746	3.23	3.212	507	-0.13	(015)
	45.43	44.75	1.996	2.023	514	0.689	(0015)
Zn _{0.3} Bi _{1.7} Te ₃	27.616	27.74	3.23	3.21	532	-0.124	(015)
	45.439	44.74	1.996	2.02	1257	0.7	(0015)

4. CONCLUSION

The XRD diffraction patterns of Bi₂Te₃ change its preferential orientation at ($2\theta = 27.79^\circ$) of [015] when alloyed by Zn elements to produce ternary alloys of Zn_xBi_{2-x}Te₃. The strongest preferential orientation at ($2\theta = 44.27^\circ$), ($2\theta = 44.75^\circ$) and ($2\theta = 44.74^\circ$) respectively of [0015] for Zn_{0.1}Bi_{1.9}Te₃, Zn_{0.2}Bi_{1.8}Te₃ and Zn_{0.3}Bi_{1.7}Te₃ as the addition of Zn element. These orientation intensities are varying according to the variation in Zn amount.

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