Research Article

Comparative Study of Substrate Type and Post-Annealing Temperature on Thermoelectric Properties of Bi_2Te_3 Thin Films

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Abstract

This study explores the effects of substrate type and post-annealing temperature on the structural and thermoelectric properties of Bi_2Te_3 thin films prepared by DC reactive magnetron sputtering. Films were deposited on both rigid (SiO_2) and flexible (polyimide, PA) substrates, followed by annealing at 50 , 150 , and 250 °C. Structural characterization via XRD and FE-SEM indicated enhanced crystallinity with increasing temperature, particularly on SiO_2, whereas films on PA exhibited minimal structural evolution due to the substrate's lower thermal stability. EDS analysis showed that annealing shifted the Bi/Te ratio closer to the stoichiometric composition, especially for SiO_2-based films. Thermoelectric measurements revealed that SiO_2-supported films consistently demonstrated lower electrical resistivity, higher Seebeck coefficient, and superior power factor compared to those on PA. The best thermoelectric performance was observed after moderate annealing on SiO_2. These results highlight the critical role of substrate selection and thermal processing in optimizing Bi_2Te_3 thin films for both rigid and flexible thermoelectric device applications.

Keywords: Thermoelectric; Bi_2Te_3 thin film; DC pulse magnetron sputtering

1. Introduction

Thermoelectric (TE) materials have attracted increasing interest in recent years due to their unique ability to directly convert waste heat into electrical energy through the Seebeck effect [1 − 2]. This energy conversion mechanism enables the development of compact, solid-state, and environmentally friendly energy harvesting systems, making TE materials highly promising for sustainable energy applications, especially in the context of energy recovery, decentralized power generation and various ambient energy sources are suitable for portable energy harvesting systems, including mechanical energy and thermal energy [3 − 4]. Among various TE materials, bismuth telluride (Bi_2Te_3) stands out as one of the most efficient and widely used compounds for near-room-temperature applications. Its favorable characteristics, including a narrow band gap (~0.13 eV), high Seebeck coefficient, and low thermal conductivity, contribute to the high thermoelectric efficiency of the material. This efficiency is typically expressed by the dimensionless figure of merit, $ZT = \sigma S2T/\kappa$, and the power factor, $PF = \sigma S2$, where σ, S, and κ denote the electrical conductivity, Seebeck coefficient, and thermal conductivity, respectively [5 – 7].

Among them, DC magnetron sputtering is widely employed due to its excellent control over film uniformity, thickness, purity, and adhesion to diverse substrates [8]. However, the thermoelectric performance of sputtered Bi_2Te_3 thin films depends not only on the deposition parameters but also significantly on post-deposition treatments, especially thermal annealing, which plays a crucial role in promoting crystallinity, grain growth, stoichiometry tuning, and carrier mobility enhancement [9]. In addition to annealing conditions, the type of substrate used during thin-film fabrication plays a critical role in determining the final film quality. Substrates influence microstructural evolution, mechanical integrity, thermal diffusion, and interface bonding, all of which directly affect thermoelectric performance. Rigid substrates such as SiO_2 wafers offer excellent thermal and structural stability, making them suitable for on-chip integration and planar TE modules [10]. Meanwhile, flexible polymer substrates like polyimide (PA) are gaining attention for their potential in wearable, conformal, and bendable TE applications [11 − 12]. Despite their flexibility, these substrates pose challenges such as limited thermal endurance and weak support for crystallization during annealing, which may degrade film quality.

Although many studies have explored Bi_2Te_3 thin films on either rigid or flexible substrates, there is a clear lack of systematic comparative research conducted under identical deposition and post-treatment conditions. This knowledge gap restricts our understanding of how substrate-dependent factors impact the structural and thermoelectric behavior of Bi_2Te_3 thin films, particularly in the context of device design that aims to bridge rigid and flexible electronics. In this work, Bi_2Te_3 thin films were deposited on both rigid (SiO_2) and flexible PA substrates using DC reactive magnetron sputtering, followed by post-annealing at various temperatures. The objective was to investigate and compare the effects of substrate type and thermal treatment on the film's morphology, crystallinity, elemental composition, and thermoelectric properties, including resistivity, Seebeck coefficient, and power factor. The findings provide meaningful insights for the optimization of Bi_2Te_3 thin films tailored for both rigid and flexible thermoelectric applications, advancing their potential for integration into next-generation energy-harvesting platforms.

2. Materials and Methods

2.1 Preparation of Bi_2Te_3 thin films

The present study presents a hybrid two-area power system consisting of a photovoltaic system and a thermal-reheat system , where the PV system is placed in area 1 of the system layout, while the thermal-reheat system is designed to be placed in area 2 of the system layout, and the system layout is shown in Fig. 1.[20]

2.2 Characterizations

The morphological and microstructural features of the Bi_2Te_3 thin films were examined using field-emission scanning electron microscopy (FE-SEM; Hitachi SU8030). Grazing incidence X-ray diffraction (GI-XRD; Rigaku TTRAX III) was employed to determine the crystallographic orientation and phase purity of the films, while energy-dispersive spectroscopy (EDS) was utilized for elemental analysis to confirm the stoichiometry of the deposited films. The electrical resistivity (ρ), Seebeck coefficient (S), and power factor (PF) of the Bi_2Te_3 thin films annealed under different atmospheres were measured using a ZEM-3 apparatus (Advance Riko) at room temperature.

3. Results and Discussions

3.1 Characterization of Bi_2Te_3 thin films

The crystallinity of Bi_2Te_3 thin films deposited on different substrates (SiO_2 and polyimide) and post-annealed at various temperatures was investigated by GI-XRD, as shown in Fig 1. For both substrates, the as-deposited films exhibit broad and low-intensity diffraction peaks, indicating a poorly crystalline or nearly amorphous structure. Upon post-annealing, a significant enhancement in crystallinity is observed, particularly at 250 °C, where a distinct peak corresponding to the (015) plane of rhombohedral Bi_2Te_3 becomes prominent [13]. This indicates the formation of a well-defined crystalline phase. The intensity and sharpness of the (015) peak increase with annealing temperature, suggesting improved atomic ordering and grain growth as thermal energy facilitates atomic diffusion and recrystallization [14 − 15]. Comparing the two substrates, the Bi_2Te_3 films on SiO_2 in Fig. 1(a) exhibit higher peak intensity and sharper diffraction features than those on polyimide Fig. 1(b) under the same annealing conditions. This implies that the rigid and thermally stable SiO_2 substrate provides a more favorable surface for crystalline growth compared to the flexible polyimide substrate, which may limit crystallization due to its lower thermal stability and surface energy. These results demonstrate that both annealing temperature and substrate type play critical roles in determining the crystallinity of Bi_2Te_3 thin films, which in turn can influence their electrical and thermoelectric properties. The average crystallite size was determined from all diffraction peaks using Scherrer's formula [16].

$$D = K\lambda / B\cos\theta \quad (1)$$

Where D is the crystallite size, K is the shape factor (0.9 for spherical particles), λ is the X-ray wavelength of Cu $K\alpha_1$ radiation (1.54059 Å), B is the full width at half maximum (FWHM) in radians, and θ is the Bragg diffraction angle. The FWHM values obtained from Gaussian fitting were applied to estimate the crystallite sizes for individual planes. The results revealed that, on SiO_2 substrates, the crystallite size of Bi_2Te_3 thin films increased with annealing temperature, ranging from 4.38 – 11.00 nm, as summarized in Table 1. In contrast, films deposited on polyimide substrates exhibited a decrease in crystallite size with increasing annealing temperature. This unusual trend can be explained by the significant mismatch in the coefficients of thermal expansion (CTE) between Bi_2Te_3 and polyimide. During film deposition and post-annealing, the polyimide substrates undergo shrinkage, inducing strain accumulation in the films, which in turn suppresses crystal growth [17 – 19]

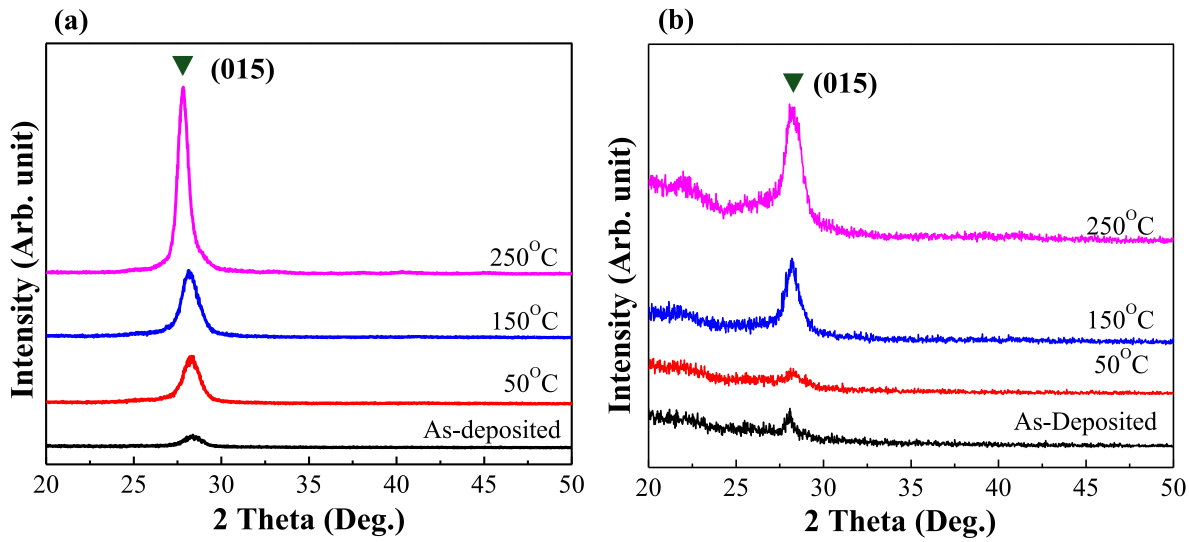

Fig. 1 Crystallinity of all Bi_2Te_3 thin films on different substrates. (a) on SiO_2 (b) on polyimide.

Table 1 Grain sizes of Bi_2Te_3 thin films calculated using GI-XRD patterns.

Condition	(015) Plane 2θ (º)	FWHM β (º)	β cosθ	Grain size D (nm)
On SiO_2 Substrate				
As-deposited	28.38	1.870	0.03264	4.38
Annealed 50ºC	28.30	1.067	0.01905	7.51
Annealed 150ºC	28.16	1.091	0.01863	7.68
Annealed 250ºC	27.82	0.741	0.01293	11.00
On Polyimide Substrate				
As-deposited	28.08	0.490	0.00855	16.70
Annealed 50ºC	28.12	0.701	0.01223	11.70
Annealed 150ºC	28.20	0.852	0.01487	9.62
Annealed 250ºC	28.06	1.034	0.01805	7.93

Fig. 2 presents the surface morphologies of Bi_2Te_3 thin films deposited on SiO_2 and PA substrates and subsequently annealed at different temperatures ranging from 50 – 250 °C. All images were captured by FE-SEM at the same magnification, enabling direct comparison of grain structure and surface features across different conditions. For the SiO_2 substrate Fig. 2(a), the as-deposited film exhibits a dense and uniform grain structure with well-defined polygonal grains. Interestingly, as the annealing temperature increases to 50, 150, and 250°C, the surface morphology remains largely unchanged. While XRD analysis in Fig. 1 indicates improved crystallinity at higher annealing temperatures, these changes are not strongly reflected in the grain structure at the surface level, suggesting that crystallographic ordering may occur predominantly in the film's interior or at the atomic scale without significantly altering the surface grain shape or size [20]. Similarly, the films deposited on PA substrates Fig. 2(b) exhibit comparable surface morphologies, both before and after thermal annealing. The grain structure on PA appears nearly identical to that observed on SiO_2, even after heat treatment at elevated temperatures. This implies that, under the current deposition and annealing conditions, the substrate type has minimal influence on the surface grain structure of Bi_2Te_3 films. These observations suggest that the Bi_2Te_3 thin films develop a consistent surface morphology regardless of substrate type (rigid or flexible) and that annealing, while improving crystallinity as confirmed by XRD, does not lead to significant grain coarsening or surface restructuring. This consistency in morphology may be beneficial for applications that require uniform film surfaces on both rigid and flexible platforms, such as wearable thermoelectric devices.

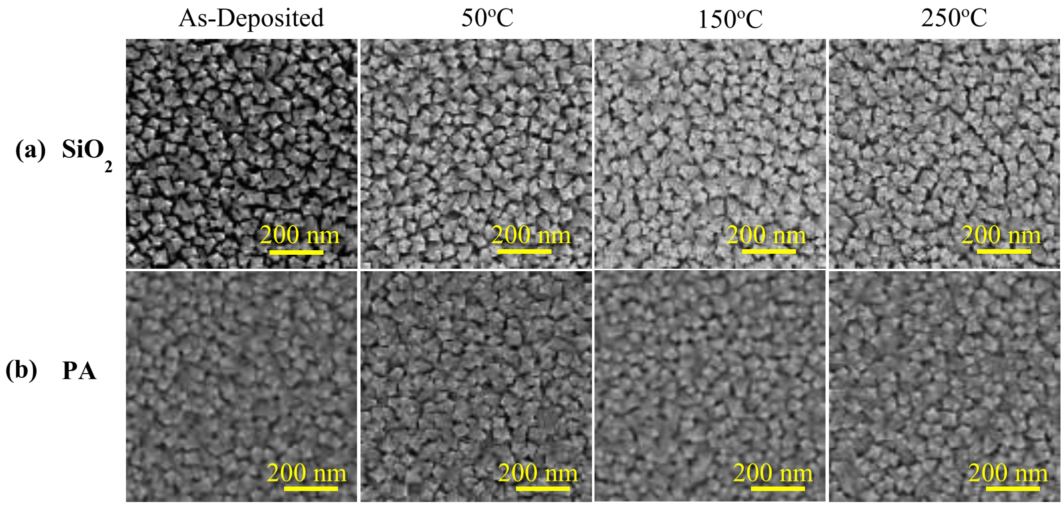

Fig. 2 The surface image morphologies of Bi_2Te_3 as-deposited and varies annealed 50 – 250 °C on different substrates.

The cross-sectional morphologies of Bi_2Te_3 thin films deposited on SiO_2 substrates and annealed at various temperatures are shown in Fig 3. The film thickness of the as-deposited sample was measured to be 304.56 ± 6.33 nm, and it slightly decreased with increasing annealing temperature. This slight reduction in film thickness may be attributed to atomic rearrangement and densification during thermal treatment. As the annealing temperature increases, enhanced atomic mobility promotes better grain packing and reduced intergranular voids, resulting in thinner and denser films [21]. Moreover, thermal energy may facilitate partial re-evaporation of the more volatile Te atoms, further contributing to the reduction in thickness. [22]

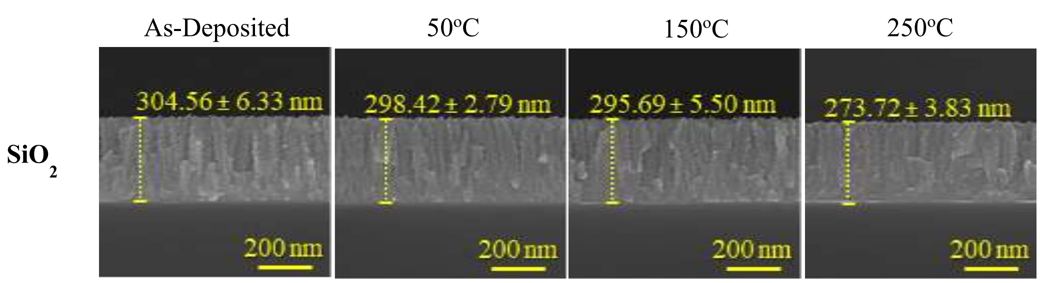

Fig. 3 The cross-section morphologies of Bi_2Te_3 as-deposited and varies annealed 50 – 250 °C on SiO_2 substrate.

Fig. 4 shows typical EDS spectra of Bi_2Te_3 thin films deposited on SiO_2 and polyimide substrates and annealed at 50 °C, 150°C, and 250°C. As expected, Bi and Te are the dominant elements, while small amounts of C and O are also detected due to surface contamination and oxidation. Table 1 summarizes the normalized atomic concentrations and Bi/Te ratios. On SiO_2 substrates, the as-deposited film shows a Te-rich composition (Bi/Te = 0.46), which becomes more stoichiometric upon annealing, reaching 0.53 at 250 °C due to Te re-evaporation at high temperatures [17]. In contrast, films on polyimide exhibit more stable Bi/Te ratios (0.49 – 0.52) across all annealing conditions, likely due to differences in substrate thermal properties affecting atomic diffusion. These results confirm that both annealing temperature and substrate type influence film composition, with annealing promoting stoichiometric adjustment, particularly on SiO_2, which may benefit crystallinity and thermoelectric performance.

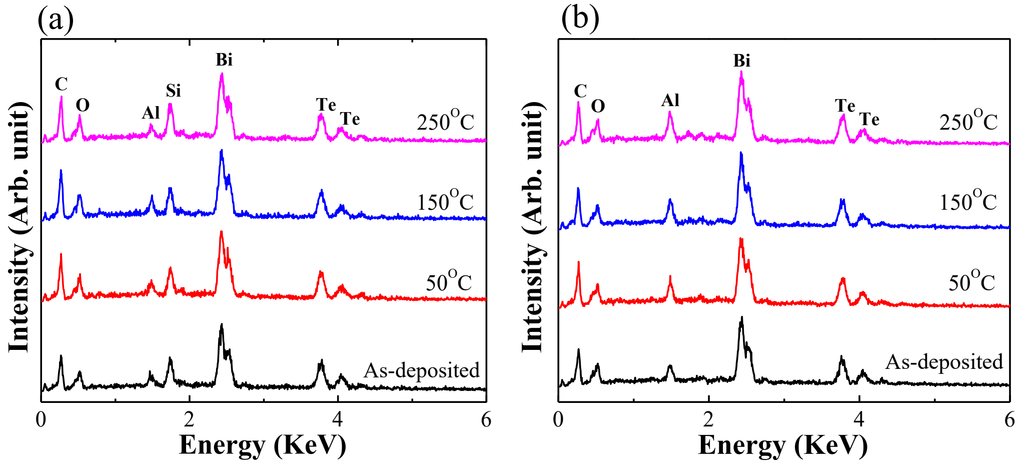

Fig. 4 EDS spectra of all Bi_2Te_3 thin films on different substrates. (a) on SiO_2 (b) on polyimide.

Table 1 Film composition of Bi_2Te_3 thin films both as-deposited and post-annealed on different substrates.

Sanple	Normalized Concentration (at.%)		
	Bi	Te	Bi/Te
SiO_2 Substrate			
As-deposited	31.66	68.33	0.46
50°C	33.74	66.25	0.50
150°C	34.35	65.64	0.52
250°C	34.75	65.24	0.53
Polyimide Substrate			
As-deposited	34.03	65.96	0.51
50°C	34.58	65.41	0.52
150°C	33.09	66.90	0.49
250°C	33.82	66.17	0.51

Fig. 5 presents the thermoelectric properties of Bi_2Te_3 thin films deposited on SiO_2 and polyimide (PA) substrates, as a function of annealing temperature. The parameters analyzed include electrical resistivity (ρ), Seebeck coefficient (S), and power factor ($PF = S^2/\rho$). In Fig. 5(a), the electrical resistivity of the SiO_2-based films shows a non-monotonic trend, with the lowest value observed after annealing at 150 °C. This behavior is likely due to improved crystallinity and carrier mobility after moderate thermal activation. At higher temperatures (250 °C), resistivity increases slightly, possibly due to increased defect formation or Te loss. In contrast, films on PA substrates exhibit relatively high and stable resistivity across all annealing temperatures, likely due to lower crystallinity and higher disorder caused by the flexible and thermally less stable nature of the polymer substrate [23]. Fig. 5(b) shows the Seebeck coefficient trends, where SiO_2-based films consistently exhibit higher S values than those on PA substrates across all annealing temperatures. This suggests better carrier energy filtering and electronic structure development on the rigid SiO_2 surface. As illustrated in Figure 5c, this advantage translates into significantly higher power factor (PF) values for SiO_2 - based films, with the peak performance observed after annealing at 50 °C. This indicates that moderate thermal treatment enhances thermoelectric efficiency, likely due to improved crystallinity and optimized carrier transport. In contrast, PA-based films exhibit low and relatively unchanged PF values, suggesting that the flexible nature of the polymer substrate limits grain growth and structural ordering, thereby suppressing thermoelectric performance. Overall, these results clearly demonstrate that both substrate type and annealing temperature play crucial roles in determining the thermoelectric behavior of Bi_2Te_3 thin films.

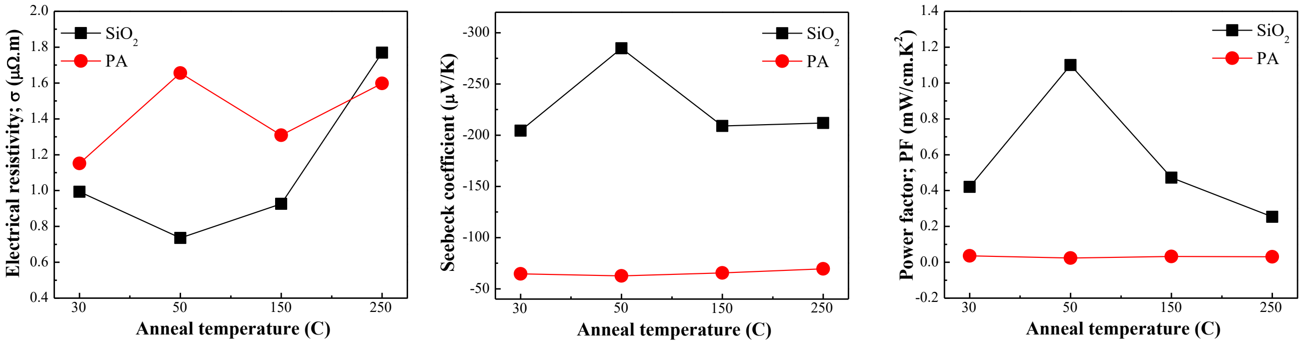

Fig. 5 Thermoelectric properties of Bi_2Te_3 thin films on all substate showed (a) electrical resistivity (b) Seebeck coefficient and (c) power factor.

Part of the experimental results This research presents an optimized controller. The controller parameters are adjusted by HO, PSO, WCA, and GWO for performance comparison. It is equipped with a thermal reheat turbine and a PV grid system. The response to a load change of 0.1 pu occurring in Area-2 (thermal reheat power system) at 0 s is simulated. The controller values are adjusted by HO, PSO, WCA, and GWO for efficiency comparison. The experiments are conducted through the program. MATLAB/Simulink on an Acer Predator laptop running 64-bit OS with an Intel® Core™ i9-13900HX processor and 32 GB DDR5 5600 MHz of RAM. The optimization procedure consisted of 10 runs with 50 populations and 50 iterations, as shown in Fig. (5).

4. Conclusion

In this study, Bi_2Te_3 thin films were successfully deposited on both rigid (SiO_2) and flexible (polyimide) substrates using DC reactive magnetron sputtering, followed by post-annealing at various temperatures. The effects of substrate type and annealing temperature on the films' structural, compositional, and thermoelectric properties were systematically investigated. XRD and FE-SEM analyses confirmed that annealing improved the crystallinity of the films, especially on SiO_2 substrates. EDS and compositional analysis revealed that post-annealing drove the Bi/Te ratio closer to the stoichiometric composition, particularly on SiO_2, due to partial Te re-evaporation at elevated temperatures. SiO_2 exhibited better thermoelectric performance, with lower resistivity, higher Seebeck coefficient, and higher power factor, particularly after moderate annealing. In contrast, films on polyimide showed limited improvement due to the substrate's low thermal stability. These findings demonstrate that both substrate rigidity and annealing control are critical to optimizing Bi_2Te_3 thin films for thermoelectric applications. Rigid substrates like SiO_2 are particularly favorable for achieving high-performance thin-film thermoelectric devices.

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