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## Performance improvement of a thin film thermoelectric generator via optimisation of the deposition parameters

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Thin film thermoelectric generators (TEGs) offer a compact and scalable solution for harvesting waste heat in microelectronic and flexible systems. However, their performance is highly influenced by material properties, fabrication parameters, and device geometry. This work presents a systematic optimization of  $\text{Bi}_2\text{Te}_3$  and  $\text{Sb}_2\text{Te}_3$  thin films for a high-performance TEG. The thin films were deposited via radio frequency (RF) magnetron sputtering under varying power conditions and characterized using XRD, FESEM, EDX, Hall measurements, and Seebeck coefficient analysis. The optimal sputtering powers were identified as 75 W for  $\text{Bi}_2\text{Te}_3$  and 30 W for  $\text{Sb}_2\text{Te}_3$ , yielding high crystallinity and balanced electrical conductivity with favourable Seebeck values. A thin film TEG consisting of six n-type/p-type leg pairs was fabricated using these conditions and subjected to post-deposition annealing to improve performance. The TEG annealed at 200 °C demonstrated a peak power output of 0.84  $\mu\text{W}$  at  $\sim 120$  °C  $\Delta T$ , indicating enhanced crystallinity and reduced internal resistance. Dimensional optimization further revealed that wider and shorter TE legs significantly improve the output by minimizing internal resistance. The results highlight the importance of integrating material, process, and device-level optimization for the development of efficient and scalable thin film thermoelectric systems.

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## 1. Introduction

The universal quest for sustainable and efficient energy technologies has intensified interest in thermoelectric generators (TEGs), which offer a direct, solid-state method for converting thermal energy into electricity.<sup>1–6</sup> Among various energy conversion technologies, thermoelectrics stand out due to their reliability, lack of moving parts, and ability to harvest low-grade waste heat,<sup>7,8</sup> making them highly attractive for applications ranging from industrial energy recovery to autonomous sensors and wearable devices.

Bismuth telluride ( $\text{Bi}_2\text{Te}_3$ ) and antimony telluride ( $\text{Sb}_2\text{Te}_3$ ) are among the most extensively studied thermoelectric materials for near-room-temperature applications, owing to their high Seebeck coefficients, moderate electrical conductivity, and inherently low thermal conductivity.<sup>9,10</sup> The efficiency of a thermoelectric

material is governed by its figure of merit ( $ZT$ ), which is strongly influenced by electrical conductivity ( $\sigma$ ), Seebeck coefficient ( $S$ ), and thermal conductivity ( $\kappa$ ), defined as  $ZT = (S^2\sigma T)/\kappa$ , where  $S^2\sigma$  can be defined as power factor ( $PF$ ). Numerous studies have focused on enhancing the thermoelectric performance to widen its potential and application. Recent efforts have shifted toward thin-film configurations, where these properties can be finely tuned through nanoscale control, improved carrier mobility, and phonon scattering mechanisms. Compared to bulk counterparts, thin-film TEGs offer several advantages, including enhanced power density, mechanical flexibility, and better integration with microelectronic and wearable systems.<sup>11,12</sup>

However, achieving optimal performance in thin-film TEGs requires a multifaceted approach. Key factors such as sputtering parameters, post-deposition treatments, and geometric design must be precisely engineered to maximize electrical output while minimizing internal resistance and thermal losses. Recent advances in  $\text{Bi}_2\text{Te}_3$  and  $\text{Sb}_2\text{Te}_3$  thin films have demonstrated that careful control of film microstructure, stoichiometry and strain can markedly improve thermoelectric performance. For example, Zheng *et al.*<sup>13</sup> demonstrated a textured, flexible  $\text{Bi}_2\text{Te}_3$  thin-film design that achieved record room-temperature  $ZT$  values ( $\sim 1.2$ ) while retaining mechanical

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robustness, underscoring the importance of crystallographic texture and film processing. In  $\text{Sb}_2\text{Te}_3$ -based systems, strategies such as lattice-strain engineering and heterostructuring have been shown to enhance the Seebeck coefficient and power factor by modifying carrier scattering and phonon transport.<sup>14</sup> Other than that, Haidar *et al.*<sup>15</sup> investigated the effects of sputtering temperature, co-sputtering techniques, and annealing treatments on the structural and thermoelectric properties of these materials for micro-scale TEGs. While their work provides valuable insights into the material-level optimization for vertical  $\mu$ TEG architectures, it does not address planar thin-film device configurations. Nevertheless, collectively, these material-level developments motivate our integrated experimental study to optimize  $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$  thin film TEG performance.

Prior studies have shown that device geometry can strongly influence output power and power density. Kalil *et al.*<sup>16</sup> conducted a detailed performance comparison of bulk TEGs by analyzing different leg geometries under constant leg volume, demonstrating that variations in leg shape and aspect ratio significantly affect power output and thermal management. However, their study focuses exclusively on bulk TEGs, where heat flow and mechanical constraints differ considerably from those in thin-film systems. Several studies combine numerical optimization with experiments to identify optimal leg geometries for thin film or wearable TEGs. For instance, Kuang *et al.*<sup>17</sup> investigated annular thin film TEG architectures and highlighted the combined role of material properties and geometry on device performance, reporting that annealing improves the film Seebeck coefficient and conductivity, while geometry sets the achievable output power density. Mathematical and numerical studies by Newbrook *et al.*<sup>18</sup> further showed that fill factor and interconnect conductivity critically determine thin film TEG performance. Building on this line of work, this study extends the understanding of thin film TEG design by focusing on planar devices, fabricated using optimized sputtering and annealing conditions, and introduces dimensional optimization of the thermoelectric legs.

In this work, we present a comprehensive investigation on the optimization of the deposition parameters for the fabrication of  $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$  thin film TEGs. This study explores the influence of sputtering power on film crystallinity and thermoelectric properties, the impact of post-deposition annealing on device performance, and the role of leg geometry in enhancing power output. By systematically examining each of these factors, this research aims to establish a set of process guidelines for the fabrication of high-performance thin film thermoelectric devices, contributing towards the development of a scalable and cost-effective energy harvesting solution.

## 2. Materials and methods

### 2.1. Deposition of thermoelectric films

$\text{Bi}_2\text{Te}_3$  and  $\text{Sb}_2\text{Te}_3$  thin films were deposited using RF magnetron sputtering on soda lime glass (SLG) substrates that were ultrasonically cleaned with methanol, acetone, ethanol, and

deionized water for 10 min. Nitrogen gas, a hot plate, and a UV ozone cleaner were also used to eliminate residues from the substrates. A sputter target of  $\text{Bi}_2\text{Te}_3$  (diameter 50.8 mm, thickness 4.25 mm, 99.999% purity) and  $\text{Sb}_2\text{Te}_3$  (diameter 50.8 mm, thickness 6.35 mm, 99.999% purity), with argon gas (99.99% purity), were used for the sputter coating. The samples were deposited without substrate heating using RF powers of 75, 90, 105, 120, and 135 W (labelled as A1, B1, C1, D1, and E1) for  $\text{Bi}_2\text{Te}_3$  at a deposition time of 60 min, and 10, 20, 30, 40, and 50 W (labelled as A2, B2, C2, D2, and E2) for  $\text{Sb}_2\text{Te}_3$  at 120 min. A longer deposition time was required for  $\text{Sb}_2\text{Te}_3$  due to the lower RF power limit imposed by the sputtering system. Due to the semiconducting nature and low thermal conductivity of  $\text{Sb}_2\text{Te}_3$ , operating at high RF power sputtering leads to localized heating at the target surface.<sup>19</sup> In our system, insufficient cooling at the sputter gun further worsened this issue, resulting in thermal instability and risk of target degradation. Therefore, a lower power range was used with an extended deposition time to achieve a film thickness comparable to that of the  $\text{Bi}_2\text{Te}_3$  layer. Although film thickness is a critical factor influencing thermoelectric performance, particularly in thin film configurations, a detailed investigation of its effect lies beyond the current scope of this study. The details of the deposition protocol are extensively discussed in our previous work.<sup>20</sup>

X-ray diffraction (XRD, X'pert-pro PANalytical X-ray diffractometer) using  $\text{Cu K}\alpha$  radiation ( $\lambda = 1.5406 \text{ \AA}$ ) was used to investigate the phase structure of all the as-deposited thin films. Rietveld refinement of the experimental XRD data was done to calculate lattice parameters  $a$  and  $c$ . The field-emission scanning electron microscopy (FESEM/JEOL, JSM7800F, operating at 3.0 kV) topographic and cross-sectional images were used to evaluate the surface microstructure and film thickness. Energy dispersive X-ray spectroscopy (EDX) attached to the FESEM was used to confirm the film composition. Moreover, the Hall effect measurement system (HMS ECOPIA 3000) with a fixed magnetic field of 0.57 T was employed to test the carrier concentration and electrical conductivity. The temperature-dependent in-plane  $S$  was measured using a Linseis LSR-3, with rectangular samples (about 2 cm  $\times$  1.25 cm) mounted for measurement. The absolute  $S$  was determined in a two-contact configuration relative to a Pt standard, applying a temperature gradient of approximately 25 °C.

### 2.2. Fabrication of the $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$ thin film TEG

The TEG consists of 6 pairs of n-type  $\text{Bi}_2\text{Te}_3$  and p-type  $\text{Sb}_2\text{Te}_3$  materials, fabricated under the optimal conditions based on the above experiments, with  $\text{Bi}_2\text{Te}_3$  deposited at 75 W for 60 min, while  $\text{Sb}_2\text{Te}_3$  at 30 W for 120 min. The TE legs were deposited on a rectangular SLG substrate of 1 mm thickness. A Kapton mask was applied to define specific deposition areas and then n-type  $\text{Bi}_2\text{Te}_3$  was deposited *via* sputtering. A second Kapton mask was applied to enable the subsequent deposition of p-type  $\text{Sb}_2\text{Te}_3$  legs in the alternating region. Finally, metallic silver (Ag) contacts were deposited to electrically connect the TE legs, completing the TEG structure (refer Fig. 2(a)). The mask-assisted sequential deposition ensures precise patterning and



alignment of thermoelectric elements and contacts. The complete process flow of TEG fabrication is described in detail in our previous work.<sup>21</sup>

**2.2.1. Post-deposition annealing of the of  $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$  thin film TEG.** A TEG consisting of legs with a standard design based on Isotta *et al.*<sup>8</sup> (2022) (width of 3 mm and length of 15 mm on a 7.6 cm × 2.5 cm substrate) was used to study the effect of post-deposition annealing on the performance of the TEG. The same TEG sample was annealed sequentially at 100 °C followed by 200 °C, allowing for the evaluation of progressive thermal effects on the same device. A tube furnace was used to anneal the TEG, purged with nitrogen to establish an inert atmosphere, and the sample was then annealed under vacuum conditions. The furnace temperature was increased gradually at a rate of 10 °C per minute until the desired annealing temperature was reached. Each temperature set was maintained for 60 minutes to allow for controlled thermal processing.

**2.2.2. Dimensional optimization of the of  $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$  thin film TEG.** To investigate the effect of geometry on device performance, several dimensional variations of the thin film TEG were designed using only  $\text{Sb}_2\text{Te}_3$  as the thermoelectric material. Four alternative patterns were fabricated with respect to the standard design: pattern I reduced the leg width to 1.5 mm; pattern II increased the width to 4.5 mm; pattern III extended the leg length to 25 mm; and pattern IV further increased the length to 35 mm (refer to Fig. 1). These variations were designed to evaluate how changes in leg width and length affect thermal and electrical resistance, and ultimately, power

output. This dimensional study enables the identification of optimal TEG leg geometry for improved device efficiency.

### 2.3. Performance analysis of the thin film TEG

Open-circuit voltage ( $V_{oc}$ ) as a function of temperature difference ( $\Delta T$ ) and current–voltage–power (IVP) characteristics were recorded using a custom setup shown in Fig. 2(c). A hot plate was used as the heat source, and a metal plate was used as the heat sink (without active cooling). All performance measurements were conducted under ambient conditions; the voltage generated by the devices was measured using a Keithley Agilent 34401A voltmeter, and temperature differences were monitored using a Fluke Ti32 thermal camera. The  $T_h$  and  $T_c$  values were taken near the TE legs as shown in Fig. 2(b). For the IVP measurement, a FLUKE 8846A (ammeter) and a variable resistor were added. All measurements were performed under a fixed temperature gradient, with the hot side maintained at approximately 150 °C and the cold side left to cool passively. The power curve of the TEG was derived and plotted using  $P = VI$  after  $I$ – $V$  values were recorded across a range of resistances.

## 3. Results and discussion

### 3.1. Characterization of $\text{Bi}_2\text{Te}_3$ and $\text{Sb}_2\text{Te}_3$ thin films

The phase purity and crystallinity of the thin films were measured using the X-ray diffraction (XRD) technique. The “substrate” curve represents the diffraction pattern of the bare substrate, confirming that other peaks observed in the spectra

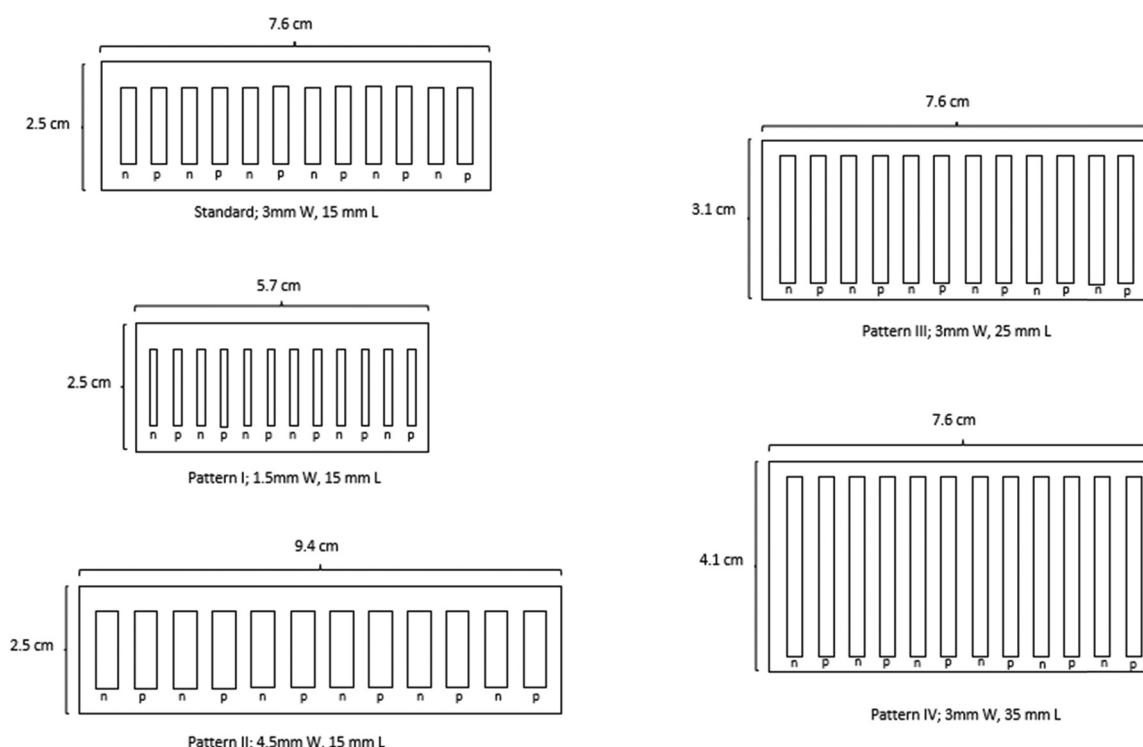


Fig. 1 Illustration of the dimension variation tested for the  $\text{Sb}_2\text{Te}_3$ -only thin film TEG.



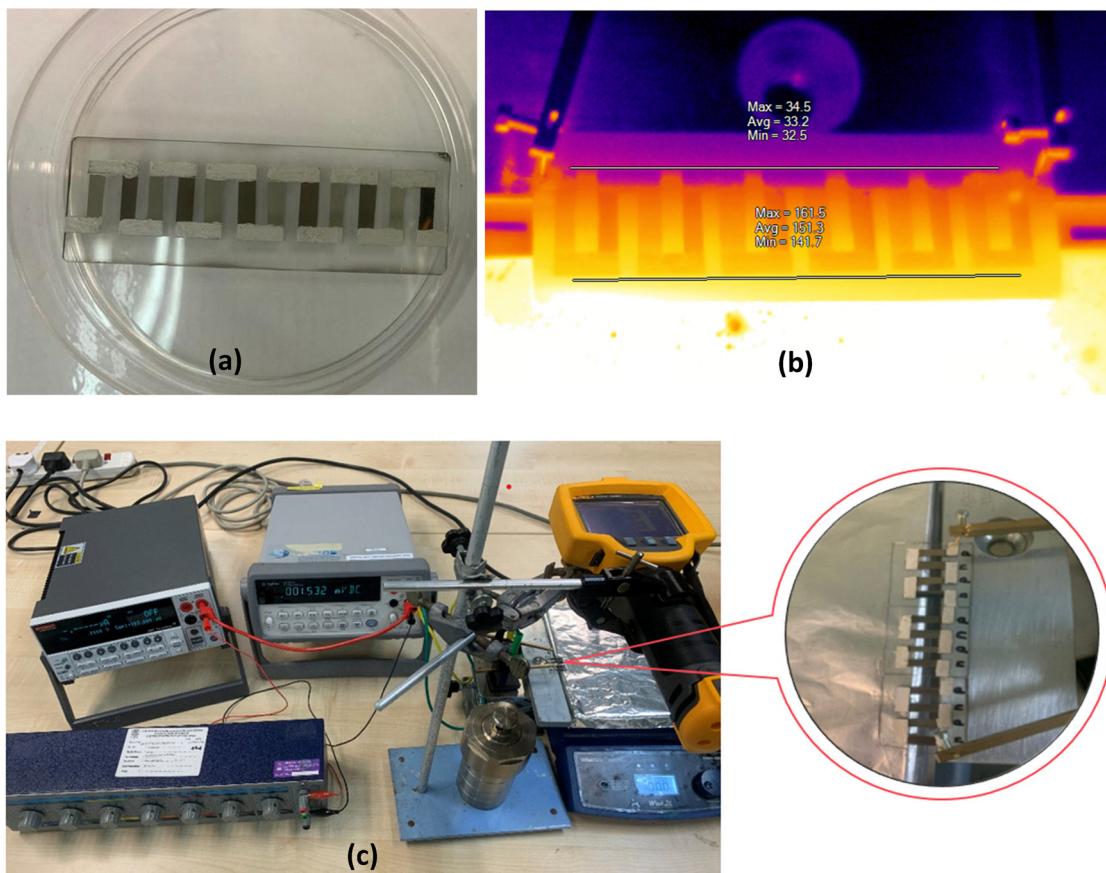


Fig. 2 (a) The fabricated  $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$  thin film TEG. (b) Thermal image of a  $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$  thin film TEG in operation. (c) Picture of the custom IVP measurement setup.

for the films are attributed to the sample layers and not the substrate. As shown in Fig. 3(a), the XRD measurements indicate a good phase purity for  $\text{Bi}_2\text{Te}_3$  samples, with no measurable trace of secondary phases. This indicates effective control over the stoichiometry and phase during the deposition process. The XRD reflections observed for  $\text{Bi}_2\text{Te}_3$  can be indexed with the respective rhombohedral  $\text{Bi}_2\text{Te}_3$  phase (PDF #00-015-0863) in the space group  $R\bar{3}m$  (166) with lattice parameters  $a = 4.3852 \text{ \AA}$  and  $c = 30.4830 \text{ \AA}$ . The observed reflections illustrate preferential growth along the  $c$ -axis with a sharp dominant peak growing anisotropically along the  $(0\ 1\ 5)$  direction, indicating a highly crystalline structure with a few small peaks corresponding to the  $(0\ 0\ 6)$ ,  $(1\ 0\ 10)$  and  $(1\ 1\ 0)$  directions. The intensity of these peaks systematically increases with RF power, indicating enhanced crystallinity as the RF power increases from 75 W to 135 W. This trend suggests that a higher RF power provides sufficient energy to atoms, promoting surface mobility and the formation of larger, well-ordered grains. This trend can also be seen more clearly in the  $\text{Sb}_2\text{Te}_3$  spectra.

For  $\text{Sb}_2\text{Te}_3$  samples (Fig. 3(b)), the peaks aligned well with the respective rhombohedral  $\text{Sb}_2\text{Te}_3$  phase (PDF #01-071-0393) in the space group  $R\bar{3}m$  (166) with lattice parameters  $a = 4.2640 \text{ \AA}$  and  $c = 30.4580 \text{ \AA}$ . The absence of extraneous peaks in the spectra confirmed that the films are phase-pure  $\text{Sb}_2\text{Te}_3$  with no

detectable secondary phases or impurities. The peaks are relatively small and broad, corresponding to the  $(0\ 1\ 5)$  direction especially at a low RF power due to the low thickness of the film, as proven by the FESEM cross-section image to be discussed. The intensity of these peaks also increases with RF power from 10 W to 50 W. At lower powers, the peaks are broader and less intense, reflecting poorer crystallinity and smaller crystallite sizes. In contrast, the peaks at 50 W are the sharpest with a notable increment at  $(1\ 1\ 0)$ , highlighting optimal conditions for achieving high-quality crystalline films. Overall, the systematic improvement in peak sharpness and intensity with increasing power highlights the critical role of power optimization in determining the structural properties of the films.

Table 1 presents the crystallite sizes of  $\text{Bi}_2\text{Te}_3$  and  $\text{Sb}_2\text{Te}_3$  thin films sputtered at different RF powers. A clear trend emerges where the crystallite size increases from 8.52 nm (sample A1) to 9.59 nm (sample E1) as the sputtering power is increased. This behaviour can be attributed to the higher energy imparted to the sputtered atoms at elevated RF powers, which enhances atom mobility on the substrate surface.<sup>22</sup> As a result, the atoms have more opportunity to diffuse, leading to larger grains during film growth. Although the overall differences in crystallite size are within a narrow range, even slight increases



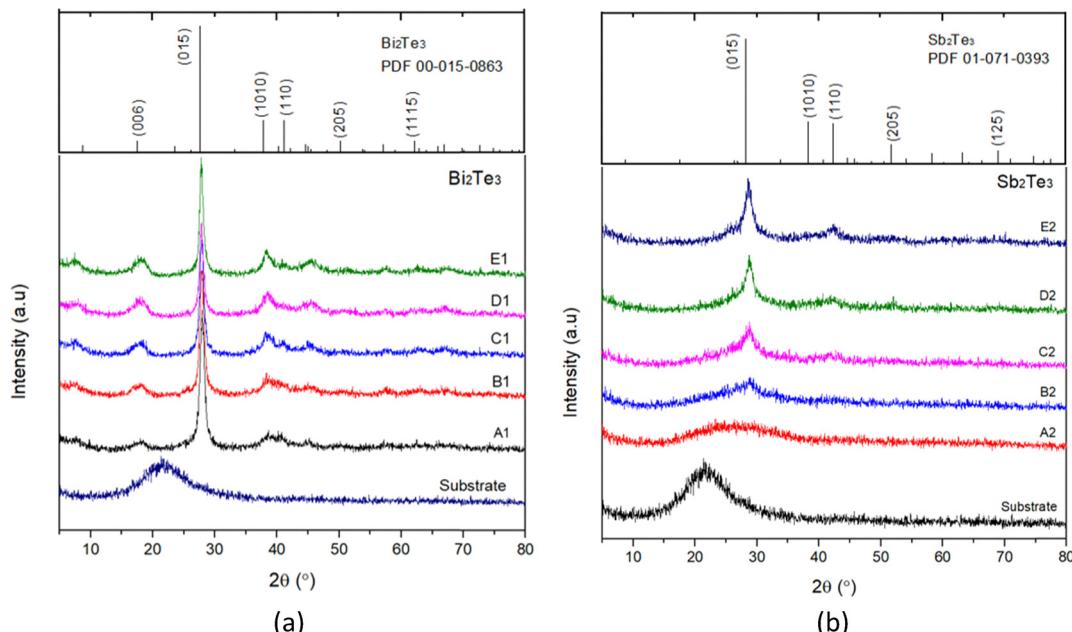


Fig. 3 XRD patterns of (a)  $\text{Bi}_2\text{Te}_3$  films deposited at 75, 90, 105, 120, and 135 W and (b)  $\text{Sb}_2\text{Te}_3$  films deposited at 10, 20, 30, 40, and 50 W.

Table 1 Crystallite size and thickness of the  $\text{Bi}_2\text{Te}_3$  and  $\text{Sb}_2\text{Te}_3$  films

Material	Sample	RF power, W	Crystallite size, nm	Thickness, $\mu\text{m}$
$\text{Bi}_2\text{Te}_3$	A1	75	8.52	1.429
	B1	90	8.57	1.742
	C1	105	8.88	1.909
	D1	120	9.46	1.945
	E1	135	9.59	2.077
$\text{Sb}_2\text{Te}_3$	A2	10	0.91	0.139
	B2	20	1.28	0.365
	C2	30	2.46	0.458
	D2	40	3.08	0.640
	E2	50	3.60	0.938

in grain size can influence the electrical and thermal properties of  $\text{Bi}_2\text{Te}_3$ . Consequently, selecting an appropriate sputtering power becomes critical for optimizing film quality and, by extension, the thermoelectric performance of the deposited layers. A similar trend emerges in the  $\text{Sb}_2\text{Te}_3$  films: the crystallite size increases from 0.91 nm (sample A2) at 10 W to 3.60 nm (sample E2) at 50 W. Compared to  $\text{Bi}_2\text{Te}_3$ ,  $\text{Sb}_2\text{Te}_3$  films exhibit notably smaller crystallite dimensions. This discrepancy can be attributed to several factors, including the lower overall power range used for  $\text{Sb}_2\text{Te}_3$  deposition, differences in material composition, and variations in growth kinetics. These results underscore the importance of tailoring sputtering parameters to each specific material system to achieve the desired microstructure and, consequently, optimal thermoelectric performance.

The FESEM micrograph shows that the as-deposited  $\text{Bi}_2\text{Te}_3$  and  $\text{Sb}_2\text{Te}_3$  films cover the entirety of the substrate in a continuous and homogenous manner. As can be seen in Fig. 4(a),  $\text{Bi}_2\text{Te}_3$  films comprise hexagonal grains, confirming the crystal structure of  $\text{Bi}_2\text{Te}_3$ . The grains are densely packed with varying sizes, indicating a polycrystalline nature. The surface of the

$\text{Sb}_2\text{Te}_3$  film (Fig. 4(b)) exhibits more fine, rounded grains and is consistent in size compared to that of the  $\text{Bi}_2\text{Te}_3$  film, indicating a nearly amorphous phase resulting in a low and broad peak in XRD. The FESEM surface images presented correspond to  $\text{Bi}_2\text{Te}_3$  deposited at 75 W for 60 minutes and  $\text{Sb}_2\text{Te}_3$  deposited at 30 W for 120 minutes. Since the surface morphology of the other films exhibited similar structural characteristics, their images are not included in the main text. Likewise, the FESEM cross-section images used for thickness estimation are omitted, as the measured values are summarized in Table 1. The complete set of FESEM images for all samples is available in the supplementary file for reference. From the cross-sectional views shown in Fig. 4(b) and (e), the interface between the film and the substrate looks distinct, suggesting good adhesion properties. The thickness of the  $\text{Bi}_2\text{Te}_3$  and  $\text{Sb}_2\text{Te}_3$  films shows a clear correlation with RF power, where a higher RF power results in increased film thickness. For  $\text{Bi}_2\text{Te}_3$ , the thickness ranges from 1.429  $\mu\text{m}$  at 75 W to 2.077  $\mu\text{m}$  at 135 W, indicating a steady increase with increasing power. Similarly, for  $\text{Sb}_2\text{Te}_3$ , the thickness increases from 0.139  $\mu\text{m}$  at 10 W to 0.938  $\mu\text{m}$  at 50 W. The observed trends are consistent with typical RF sputtering behaviour, where increased power enhances the kinetic energy of the sputtered species, leading to higher deposition rates.<sup>23,24</sup> However, while thicker films may improve mechanical stability, they can also influence electrical and thermal transport properties, which must be carefully optimized for thermoelectric applications.

The EDX spectra of both  $\text{Bi}_2\text{Te}_3$  and  $\text{Sb}_2\text{Te}_3$  thin films provide crucial insights into the elemental composition and purity of the deposited materials. In the case of  $\text{Bi}_2\text{Te}_3$ , the spectrum shows prominent peaks corresponding to bismuth (Bi) and tellurium (Te), with their respective weight percentages



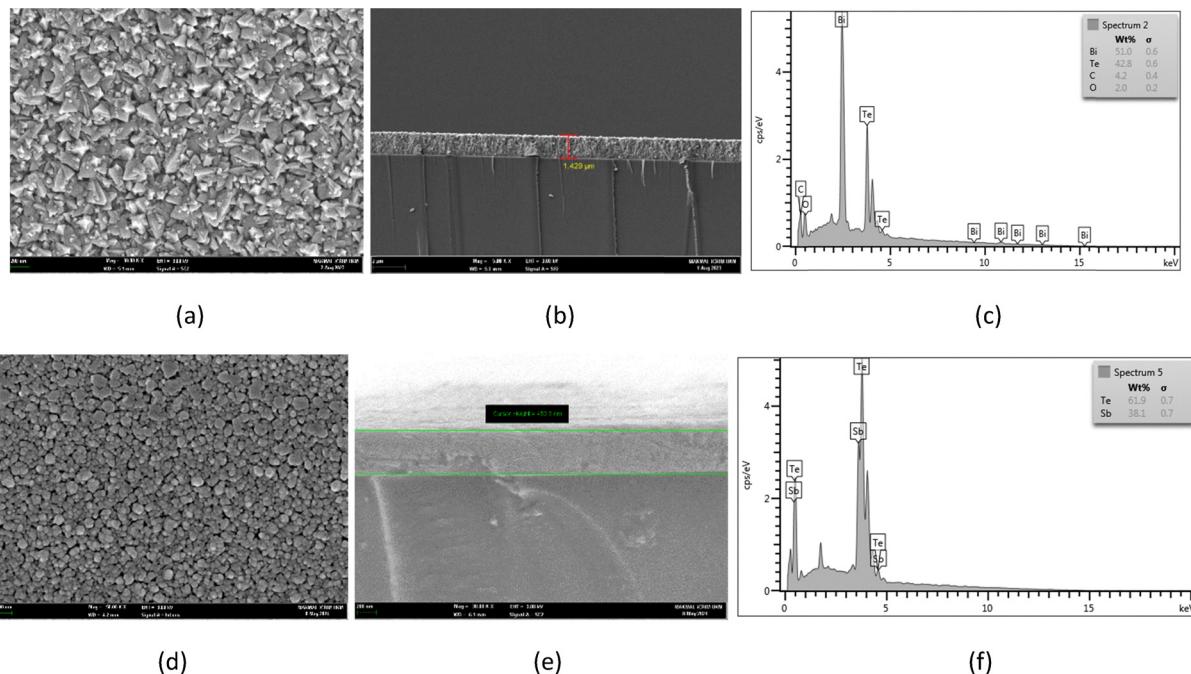


Fig. 4 FESEM surface, cross-section and EDX spectra of the (a)–(c)  $\text{Bi}_2\text{Te}_3$  and (d)–(f)  $\text{Sb}_2\text{Te}_3$  films.

of 51.0% and 42.8%. Additionally, small traces of carbon (4.2%) and oxygen (2.0%) are observed, likely due to surface contamination or oxidation. The composition of the films was calculated from the EDX spectra, shown in Fig. 4(c), giving an atomic percent of 41.9% Bi: 58.1% Te. The near-stoichiometric Bi–Te ratio suggests a well-formed  $\text{Bi}_2\text{Te}_3$  structure, which is desirable for thermoelectric applications. Similarly, the  $\text{Sb}_2\text{Te}_3$  spectrum exhibits dominant peaks of antimony (Sb) and tellurium (Te), with weight percentages of 38.1% and 61.9%, respectively. The composition of the films was calculated from the EDX spectra, shown in Fig. 4(f), giving an atomic percent of 40.0% Sb:60.0% Te. The estimated values show that the film gave a consistent Sb:Te ratio of 2:3, indicating that stoichiometric  $\text{Sb}_2\text{Te}_3$  was successfully fabricated. The EDX spectra presented here

are representative of the  $\text{Bi}_2\text{Te}_3$  and  $\text{Sb}_2\text{Te}_3$  thin films, as the atomic compositions for the other samples exhibit similar elemental distributions. Due to this consistency, the EDX results for the remaining samples are not included in the main text but will be provided in the supplementary file for reference.

### 3.2. Thermoelectric properties of the $\text{Bi}_2\text{Te}_3$ and $\text{Sb}_2\text{Te}_3$ thin films

Fig. 5(a) illustrates the variation in  $\sigma$  and carrier concentration of the deposited  $\text{Bi}_2\text{Te}_3$  thin films. Electrical conductivity, represented by the black plot, increases steadily with RF power, starting at approximately  $100 (\Omega \text{ cm})^{-1}$  for sample A1 and reaching over  $350 (\Omega \text{ cm})^{-1}$  for sample E1. This enhancement in  $\sigma$  is attributed to improvements in the structural quality of

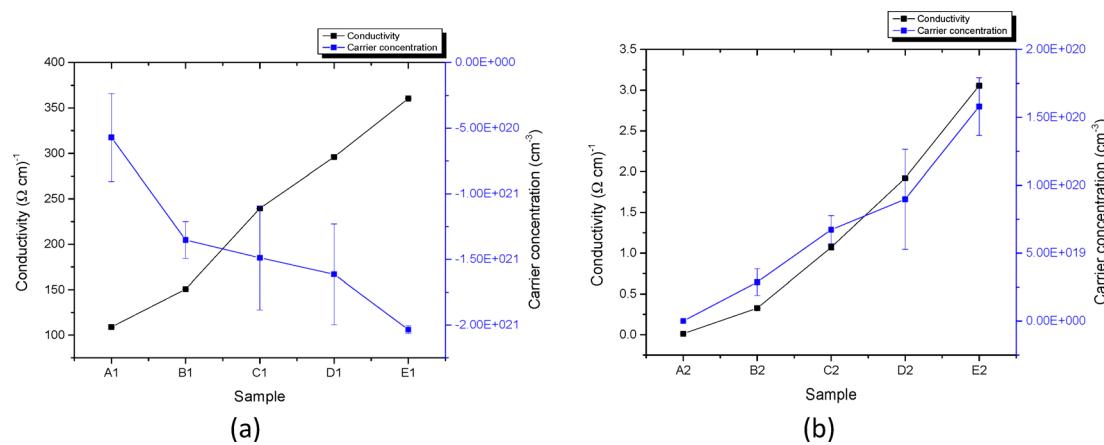


Fig. 5 Conductivity and carrier concentration of (a) n-type  $\text{Bi}_2\text{Te}_3$  (shown as negative values to indicate electron carriers) and (b) p-type  $\text{Sb}_2\text{Te}_3$  thin films.



the films, as revealed by the XRD results. At a lower RF power, the XRD spectra display broader and weaker peaks, indicating lower crystallinity and smaller grain sizes. These features increase grain boundary scattering, thereby hindering charge carrier transport.<sup>25</sup> In contrast, at a higher RF power, the diffraction peaks become sharper and more intense, reflecting improved crystallinity and larger grain sizes, which reduce grain boundary scattering and enable better charge transport. Moreover, FESEM analysis shows that film thickness increases with RF power, providing more carriers for charge conduction and further enhancing  $\sigma$ .<sup>26</sup>

The carrier concentration, represented by the blue squares, exhibits an increasingly negative trend with a higher RF power. The carrier concentration measured using Hall effect measurements is derived from the Hall coefficient ( $R_H$ ). The sign and magnitude of the Hall coefficient provide crucial information about the type and density of charge carriers present in the material.<sup>27</sup> Specifically, a positive Hall coefficient indicates that the majority charge carriers are holes, identifying the material as p-type, whereas a negative Hall coefficient signifies that majority charge carriers are electrons, indicating n-type conductivity. Hence, the negative magnitude in the figure indicates the n-type conductivity of  $\text{Bi}_2\text{Te}_3$ , and the carrier concentration value is actually increasing at a higher RF power. At a lower RF power (75 W, sample A1), the carrier concentration is approximately  $5.71 \times 10^{20} \text{ cm}^{-3}$ , and it changes to around  $2.03 \times 10^{21} \text{ cm}^{-3}$  at 135 W (sample E1).

The same trends were observed for  $\text{Sb}_2\text{Te}_3$  thin films (Fig. 5(b)). Both  $\sigma$  and carrier concentration increase consistently with a higher RF power. Specifically, sample A2 shows the lowest  $\sigma$  and carrier concentration, while sample E2 demonstrates the highest values for both parameters. The magnitude of the carrier concentration shows positive values, indicating p-type conductivity for all samples. Overall, the results confirm that increasing RF power enhances the structural and electrical properties of  $\text{Sb}_2\text{Te}_3$  thin films by improving crystallinity and increasing thickness, leading to higher  $\sigma$  and carrier concentration.

The  $S$  plot of  $\text{Bi}_2\text{Te}_3$  thin films (Fig. 6(a)) deposited at various RF powers demonstrates the dependence of thermoelectric

properties on deposition parameters. The negative values of absolute  $S$  across all samples confirmed that the films exhibit n-type conductivities, where electrons serve as the dominant charge carriers, consistent with Hall effect measurements. The  $S$  value increases with increasing temperature for all samples. This trend indicates a favourable thermoelectric response with temperature, which is associated with grain growth at elevated temperatures,<sup>28</sup> leading to reduced carrier scattering.<sup>29</sup> However, it should be noted that a comprehensive evaluation of thermoelectric performance requires consideration of electrical and thermal conductivities in addition to  $S$ .

At near room temperature, sample A1 shows the highest absolute  $S$ , approximately  $-60 \mu\text{V K}^{-1}$ , indicating superior thermoelectric performance compared to other samples. The higher magnitude of the  $S$  suggests a more significant contribution of charge carrier diffusion to the thermoelectric voltage, which is beneficial for energy conversion efficiency. The higher  $S$  of sample A1 can be correlated with its relatively lower carrier concentration, as shown in Fig. 5(a). According to the Pisarenko relation, the  $S$  is inversely related to carrier concentration, whereby a reduction in carrier density enhances the energy dependence of carrier transport and thus increases the Seebeck value.<sup>30</sup> A lower RF power during deposition resulted in a finer grain structure and a moderate carrier concentration, balancing  $\sigma$  and thermoelectric performance. In contrast, samples deposited at higher RF powers, such as sample E1, show reduced  $S$ , due to increased carrier concentrations that lower the thermoelectric voltage.

Fig. 6(b) demonstrates the  $S$  plot of  $\text{Sb}_2\text{Te}_3$  thin films, deposited using RF powers ranging from 10 W (sample A2) to 50 W (sample E2). The positive values of  $S$  for all samples confirm the p-type conductivity of the thin films, where holes act as the primary charge carriers. This observation aligns with the intrinsic behaviour of  $\text{Sb}_2\text{Te}_3$ , a well-known p-type thermoelectric material. Sample A2 exhibits an unusually high  $S$  near room temperature, exceeding the expected range, due to instrument limits. The conductivity of sample A2 is too low, falling below the resistance limit of the Seebeck instrument. As a result, the measured value lies outside the expected range,

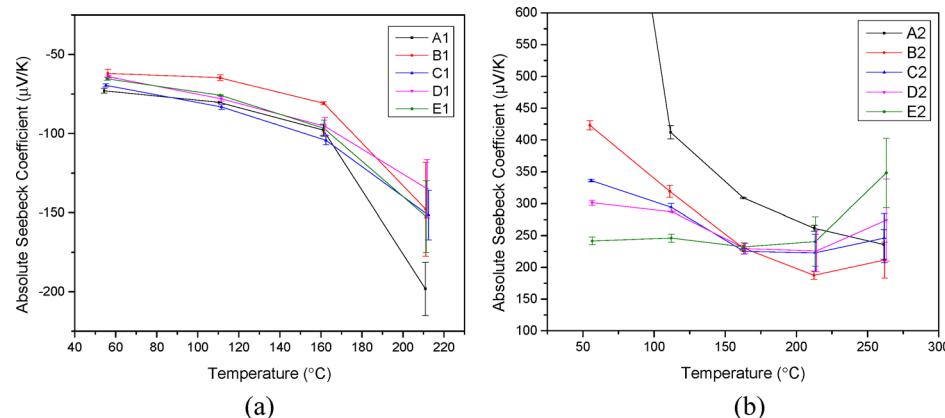


Fig. 6 Seebeck coefficient of (a)  $\text{Bi}_2\text{Te}_3$  and (b)  $\text{Sb}_2\text{Te}_3$  thin films.



making the said measurement unreliable. However, as the temperature increases, the  $S$  stabilizes and shows improved consistency, suggesting that the carrier transport mechanisms become more favourable at higher temperatures. This trend indicates a strong dependence of thermoelectric performance on the deposition conditions, with a low RF power significantly affecting carrier concentration or scattering. The  $S$  of the  $\text{Sb}_2\text{Te}_3$  thin films exhibits a distinct trend where it decreases with increasing temperature up to a certain point and then starts to increase again at higher temperatures. These results suggest a relatively stable thermoelectric performance for  $\text{Sb}_2\text{Te}_3$ , although the slight decrease indicates some temperature dependence, attributed to the amorphous–crystalline transition. Similar behaviour has also been reported by Fang *et al.*<sup>30</sup> and V. Damodara *et al.*<sup>31,33</sup>

The  $\sigma$  and  $S$  of the thin films were determined to calculate the power factor ( $PF$ ) of each film.  $PF$  becomes a decisive parameter for the selection of thin film materials due to its configuration. A low thermal conductivity is ideal for high efficiency; however, the substrate typically dominates thermal transport in thin film configurations because of the significant difference in thickness.<sup>32</sup> Table 2 shows the calculated power factors of each sample at ambient temperature.

The  $S$  and  $\sigma$  values greatly influenced the  $PF$  of thermoelectric materials, calculated by  $PF = S^2\sigma$ . However, these two properties exhibit an inverse relationship due to their mutual dependence on carrier concentration, where an increase of one promotes a decrease of the other.<sup>33</sup> The trend in the data reflects the well-known trade-off between these two properties.

For  $\text{Bi}_2\text{Te}_3$ , both  $\sigma$  and  $S$  exhibit variations across different samples, influencing the power factor. The trend shows that as conductivity increases (from  $108.96\text{ }(\Omega\text{ cm})^{-1}$  in sample A1 to  $360.46\text{ }(\Omega\text{ cm})^{-1}$  in sample E1),  $S$  generally decreases (from  $72.84\text{ }\mu\text{V K}^{-1}$  to  $65.33\text{ }\mu\text{V K}^{-1}$ ). However, this reduction in  $S$  is not steep enough to significantly lower the power factor. As a result, the power factor increases progressively from sample A1 ( $0.5781\text{ }\mu\text{W K}^2\text{ cm}^{-1}$ ) to sample E1 ( $1.5384\text{ }\mu\text{W K}^2\text{ cm}^{-1}$ ). This suggests that increasing  $\sigma$  plays a dominant role in improving the thermoelectric performance of  $\text{Bi}_2\text{Te}_3$ .

For  $\text{Sb}_2\text{Te}_3$ , the opposite trend is observed compared to  $\text{Bi}_2\text{Te}_3$ . The  $S$  is significantly higher in samples with lower  $\sigma$ , particularly in sample A2, but  $\sigma$  is very low ( $0.01067\text{ }(\Omega\text{ cm})^{-1}$ ),

leading to a very small power factor ( $0.0163\text{ }\mu\text{W K}^2\text{ cm}^{-1}$ ). As  $\sigma$  increases from sample A2 to sample E2,  $S$  decreases sharply, from  $1236.84\text{ }\mu\text{V K}^{-1}$  to  $241.56\text{ }\mu\text{V K}^{-1}$ . While  $\sigma$  increases significantly (from  $0.01067$  to  $3.055\text{ }(\Omega\text{ cm})^{-1}$ ), the strong reduction in  $S$  limits the power factor improvement. Consequently, the power factor increases but at a much lower rate than in  $\text{Bi}_2\text{Te}_3$ , reaching a maximum of  $0.1783\text{ }\mu\text{W K}^2\text{ cm}^{-1}$  in sample E2. These results highlight that optimizing thermoelectric performance depends on finding a balance between  $\sigma$  and  $S$ .

The results obtained above guide the selection of the deposition parameters for device fabrication. While certain parameters yield higher  $PF$  values, other factors such as stability, reproducibility, and temperature-dependent behavior must also be considered. Achieving a balance between these aspects ensures that the fabricated device performs efficiently across a range of operating conditions. For the fabrication of the TEG, sample A ( $\text{Bi}_2\text{Te}_3$ ) was selected due to its higher  $S$  near room temperature, which is critical for applications operating across ambient-to-moderate temperature gradients. This characteristic ensures sustained thermoelectric performance and contributes to a higher thermoelectric figure of merit ( $ZT$ ). For the  $\text{Sb}_2\text{Te}_3$  layer, sample C was chosen owing to its stable and consistent thermoelectric behaviour across the measured temperature range, offering a reliable balance between efficiency and operational stability. Although some samples exhibited higher  $PF$ , the selection was primarily guided by  $S$  trends, given that Hall measurements were limited to room temperature. The chosen samples demonstrated an optimal combination of initial  $S$  values, thermal stability, and structural integrity, ensuring enhanced efficiency, reliability, and practical applicability of the optimized TEG device.

### 3.3. Performance analysis of the $\text{Bi}_2\text{T}_3/\text{Sb}_2\text{Te}_3$ thin film TEG

In this section, the fabrication of a TEG with 6 pairs of n-type  $\text{Bi}_2\text{Te}_3$  and p-type  $\text{Sb}_2\text{Te}_3$  with optimal deposition parameters studied above is described, and its performance was analysed. The measurement of  $\Delta T$  versus  $V_{oc}$  was done in the temperature range of  $100$ – $200\text{ }^\circ\text{C}$ , with a  $10\text{ }^\circ\text{C}$  increment, although the measured  $\Delta T$ s did not fully match the set temperature of  $T_h$  and  $T_c$  due to the poor heat sink setup and heat dispersion on the hotplate. Fig. 7(a) demonstrates a linear relationship

**Table 2** Conductivity, absolute Seebeck coefficient and power factor of each sample at ambient temperature

Material	Sample	Conductivity, $\sigma$ ( $\Omega\text{ cm})^{-1}$	Absolute Seebeck coefficient, $S$ ( $\mu\text{V K}^{-1}$ )	Power factor, $PF$ ( $\mu\text{W K}^2\text{ cm}^{-1}$ )
$\text{Bi}_2\text{Te}_3$	A1	108.96	72.84	0.5781
	B1	150.6	62.02	0.5793
	C1	239.46	69.43	1.1543
	D1	295.92	64.03	1.2132
	E1	360.46	65.33	1.5384
$\text{Sb}_2\text{Te}_3$	A2	0.01067	(OOR)	
	B2	0.32594	423.43	0.1584
	C2	1.0696	336.11	0.1208
	D2	1.9206	301.44	0.1745
	E2	3.055	241.56	0.1783



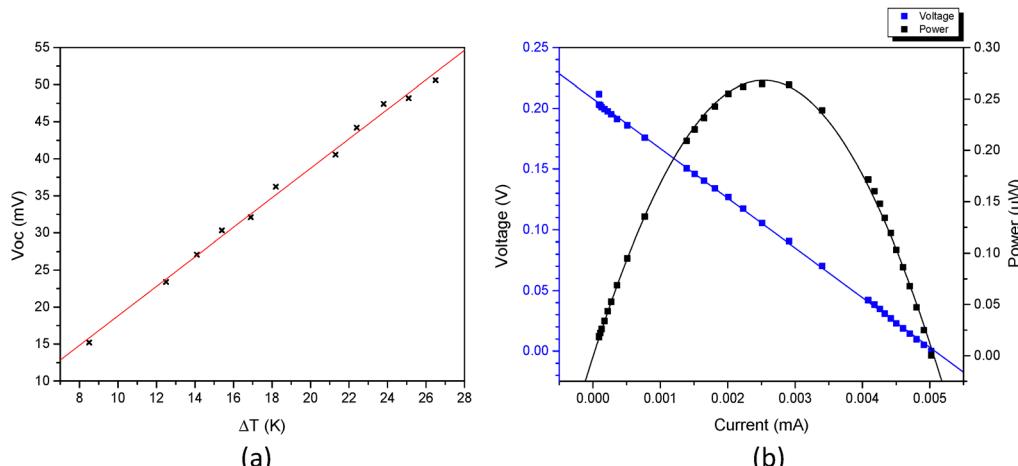


Fig. 7 (a)  $V_{oc}$  vs.  $\Delta T$  and (b) IVP plot of the optimized  $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$  thin film TEG.

between  $V_{oc}$  and the applied  $\Delta T$ , indicating the typical and ideal response of a TEG.<sup>34</sup> The steepness of the slope reflects a high  $S$ , suggesting that the TEG material efficiently converts the thermal gradient into an electrical voltage. Under these conditions, the TEG composed of 6 n-p leg pairs achieved a noteworthy maximum  $V_{oc}$  of 50.59 mV at a  $\Delta T$  of 26.5 K. Fig. 7(b) shows the current–voltage ( $IV$ ) and the current–power ( $IP$ ) curve of the optimized  $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$  thin film TEG. The  $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$  thin film TEG achieved a peak power output of 0.26  $\mu\text{W}$  at 0.0025 mA under a  $\Delta T$  of  $\sim 120$  °C. When normalized to the active planar area and number of TE legs, the maximum power density was calculated to be 0.05  $\mu\text{W cm}^{-2}$ . While this output is modest compared to vertically structured or heavily engineered TEGs, it aligns well with the performance reported for planar thin films employing comparable material systems and fabrication methods.<sup>35–38</sup>

### 3.4. Annealing effect on the performance of the $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$ thin film TEG

Fig. 8(a) shows the IV characteristics of the optimized  $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$  thin-film thermoelectric generator (TEG) annealed at

100 °C and 200 °C. The sample annealed at 200 °C (A200) shows a lower slope compared to the other conditions, indicating a lower internal resistance. This suggests that annealing at 200 °C improves  $\sigma$ , due to enhanced crystallinity and reduced grain boundary scattering.<sup>39–41</sup> On the other hand, the sample annealed at 100 °C (A100) exhibits a slightly higher resistance than the optimized sample.<sup>44</sup>

Fig. 8(b) exhibits the IP plot, illustrating the power output as a function of current for the optimized  $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$  thin-film TEG annealed at different temperatures. The curves show distinct power–current characteristics, indicating the influence of annealing temperature on the TEG's performance. Among the three samples, the TEG annealed at 200 °C (A200) exhibits the highest power output, peaking at 0.84  $\mu\text{W}$  at around 0.012 mA. This indicates that higher annealing temperatures enhance the  $\sigma$  and overall thermoelectric efficiency of the device. This improvement is due to enhanced crystallinity, reduced grain boundary scattering, and optimized carrier concentration, which collectively contribute to better charge transport properties, confirming that the reduced internal resistance contributes to improved electrical performance.

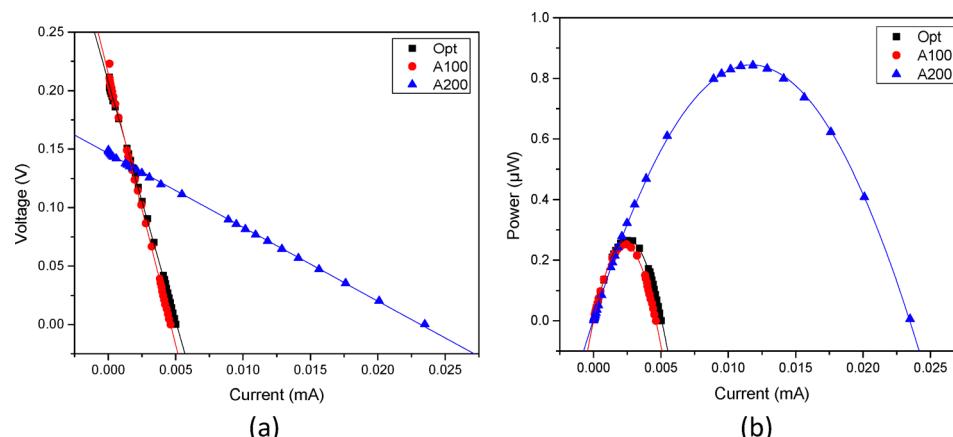


Fig. 8 (a) IV and (b) IP plots of the optimized  $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$  thin film TEG, annealed at 100 and 200 °C.



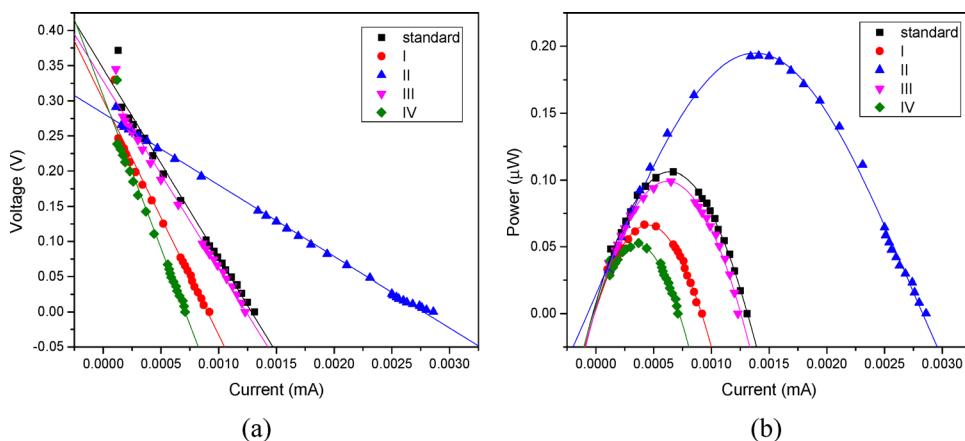


Fig. 9 (a) IV and (b) IP plots of the  $\text{Sb}_2\text{Te}_3$ -only thin film TEG with different dimensions.

In contrast, the TEG annealed at  $100\text{ }^\circ\text{C}$  (A100) demonstrates a slight reduction in power output compared to the optimized sample,  $0.25\text{ }\mu\text{W}$  at around  $0.003\text{ mA}$ , aligning with the IV results where increased resistance may have caused power dissipation. This behavior can be correlated with the  $S$  trends shown in Fig. 6, where  $\text{Bi}_2\text{Te}_3$  (sample A1) shows only a modest increase in Seebeck value when the temperature increases to  $100\text{ }^\circ\text{C}$ , while  $\text{Sb}_2\text{Te}_3$  (sample C2) experiences a more pronounced reduction. Since the overall device voltage and power are determined by the combined contributions of both p-type and n-type legs, the significant degradation in the  $\text{Sb}_2\text{Te}_3$   $S$  offsets the minor improvement in  $\text{Bi}_2\text{Te}_3$ , resulting in a net decrease in thermoelectric performance at  $100\text{ }^\circ\text{C}$ . Thus, annealing at  $200\text{ }^\circ\text{C}$  appears to optimize the material properties, leading to enhanced thermoelectric efficiency.

### 3.5. Dimensional optimization of the TEG

Fig. 9(a) shows the voltage–current characteristics of  $\text{Sb}_2\text{Te}_3$ -only thin film TEGs with different dimensions, including a standard design. All measurements were done at a  $\Delta T$  of approximately  $120\text{ }^\circ\text{C}$ . The slope of each curve represents the internal resistance of the TEG, which is influenced by the length and width of the legs. Longer legs, such as the  $25\text{ mm}$  and  $35\text{ mm}$  designs, exhibit a higher internal resistance compared to the standard  $15\text{ mm}$  legs. This is because resistance increases with length, as expressed by the formula,

$$R = \rho \frac{L}{A},$$

where  $\rho$  is the resistivity and  $A$  is the cross-sectional area. While lengthening the legs can enhance thermal resistance and broaden the temperature gradient (boosting voltage), it simultaneously increases electrical resistance, resulting in diminished output current and steeper IV slopes.<sup>42,43</sup> On the other hand, the width of the legs also plays a crucial role. The narrower  $1.5\text{ mm}$  legs exhibit higher resistance due to a smaller cross-sectional area, which restricts current flow and results in steeper IV slopes. In contrast, the wider  $4.5\text{ mm}$  legs have lower resistance, allowing more current to flow and producing a flatter IV slope. This trend

follows the inverse relationship of resistance with cross-sectional area, where a larger area reduces resistive losses.<sup>44</sup>

Fig. 9(b) shows the IP curve of  $\text{Sb}_2\text{Te}_3$ -only thin film TEGs with different dimensions. The wider leg ( $4.5\text{ mm}$ ) produces the highest power output, peaking at  $0.19\text{ }\mu\text{W}$ , due to its lower internal resistance, which allows for a higher current flow. On the other hand, narrower legs ( $1.5\text{ mm}$ ) exhibit a significantly lower power output compared to the standard dimension ( $0.11\text{ }\mu\text{W}$ ), peaking at  $0.07\text{ }\mu\text{W}$  due to their higher resistance, which restricts current flow and reduces the overall efficiency of the device. For longer legs, the maximum power is reduced,  $0.10\text{ }\mu\text{W}$  for  $25\text{ mm}$  and  $0.05\text{ }\mu\text{W}$  for  $35\text{ mm}$  compared to the standard dimensions, as their increased resistance limits current flow despite maintaining a good temperature gradient. From the IVP plot, it is evident that wider legs provide better  $\sigma$ , while longer or narrower legs increase resistance, limiting current output. The results from the dimensional optimization provided valuable and clear insights into the impact of dimension control on the performance of the TEGs, providing a crucial foundation for future research.

## 4. Conclusion

The thermoelectric properties and performance optimization of  $\text{Bi}_2\text{Te}_3$  and  $\text{Sb}_2\text{Te}_3$  thin films for TEG applications have been successfully studied. The results demonstrated that the best strategy for enhancing TEG performance involves careful control of deposition parameters, post-deposition annealing, and dimensional optimization. For  $\text{Bi}_2\text{Te}_3$  thin films, the optimal RF sputtering conditions were identified as  $75\text{ W}$  for  $60$  minutes, yielding the highest  $\sigma$  and  $S$ . For  $\text{Sb}_2\text{Te}_3$  thin films, the best results were achieved with an RF power of  $30\text{ W}$  for  $120$  minutes, balancing carrier concentration and  $\sigma$ . Post-deposition annealing at  $200\text{ }^\circ\text{C}$  further improved thermoelectric performance by enhancing crystallinity and reducing grain boundary scattering, leading to increased power output and overall efficiency. Dimensional optimization revealed that wider and shorter thermoelectric legs minimized internal resistance while maintaining effective thermal gradients, maximizing power



generation. These findings highlight the importance of a holistic approach that combines material optimization, thermal treatment, and geometric design to achieve high-efficiency TEGs. The continuation of this study should prioritize several key areas to enhance their performance and broaden their applications, such as accurately measuring the thermal conductivity of the films to understand the overall thermoelectric efficiency, systematically investigating the effect of film thickness on thermoelectric performance and exploring doping or alloying  $\text{Bi}_2\text{Te}_3$  and  $\text{Sb}_2\text{Te}_3$  with other elements, such as In or Mn, that could further optimize the  $S$ ,  $\sigma$ , and thermal stability.

## Conflicts of interest

There are no conflicts to declare.

## Data availability

The data supporting this article have been included as part of the supplementary information (SI). Supplementary information is available. See DOI: <https://doi.org/10.1039/d5ma00823a>.

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