Efficient thermoelectric (TE) conversion of waste heat to usable energy is a holy grail promising to address major societal issues related to energy crisis and global heat management. For these to be economical, synthesis of a solid-state material with a high figure-of-merit (ZT) values is the key, with characterization methods quantifying TE and heat transport properties being indispensable for guiding the development of such materials. In the present study, a large enhancement of the TE power factor in Sb$_2$Te$_3$/MoS$_2$ multilayer structures is reported. A new approach is used to simultaneously experimentally determine the values of in-plane ($k_x$) and out-of-plane ($k_z$) thermal conductivities for multilayer samples with characteristic layer thickness of few nanometres, essential for the quantification of the ZT, the key parameter for the TE material. Combining simultaneous enhancement in the value of in-plane power factor (to $(4.9 \pm 0.4) \times$ mWm$^{-1}$K$^{-2}$) and reduction of the in-plane value of the thermal conductivity (to $0.7 \pm 0.1$ Wm$^{-1}$K$^{-1}$) for Sb$_2$Te$_3$/MoS$_2$ multilayer sample led to high values of ZT of $2.08 \pm 0.37$ at room temperature. The present study, therefore, sets the foundation for a new methodology of exploiting the properties of 2D/3D interfaces for the development of novel fully viable thermoelectric materials.

1. Introduction

Two dimensional (2D) superlattice structures for thermoelectric (TE) applications are receiving increasing attention due to the possibility of enhancing the thermoelectric dimensionless figure of merit defined as $ZT = \frac{\sigma S^2 T}{\kappa}$, where $S$ is the Seebeck coefficient, $\sigma$ is the electrical conductivity, $\kappa$ is the sum of electronic and lattice thermal conductivities.$^{[1-3]}$ In a solid-state material, these three essential transport parameters are coupled owing to their direct relation with electron and phonon transport, with both linked to material atomic structure. The ZT value observed in most of the materials is quite low$^{[4,5]}$ and the primary challenge is to elevate the performance via decoupling the unfavorable interdependences between the thermal and electrical transport parameters. The idea of improving response by exploiting the quantum size effect was introduced in initial studies by Dresselhaus$^{[6]}$, Harman$^{[7]}$ and Subramanian$^{[2]}$. In recent years, several studies have been performed with an objective to enhance the response in quantum superlattice and quantum well systems.$^{[8,9]}$ The anisotropic nature of these structures has proven to be beneficial in manipulating their performance.$^{[10]}$ It has been predicted that low dimensional materials could give higher ZT values in comparison to common Sb$_2$Te$_3$ and Bi$_2$Te$_3$ layers having typical values of $ZT = 1.0$ at room temperature.$^{[3,11,12]}$ Improvement in the ZT values for superlattice and nanostructured materials is expected due to a reduction in the value of thermal conductivity. Moreover, the unique size-dependent properties or electronic structure of low-dimensional materials may also have an impact on the Seebeck coefficient and electron transport.$^{[13]}$ Recently, a ZT value of 2.6 was reported, which was observed in a single crystal SnSe sample at 900 K.$^{[14]}$ At the same time,
at this high temperature of 900 K, several competitive methods are available for use in power generation, which possess higher efficiencies. Therefore, a material having a high figure of merit in the moderate temperature range (i.e., 300–500 K) would be extremely useful for power generation. At present, the Bi$_2$Te$_3$/Sb$_2$Te$_3$ superlattice structure fabricated using the molecular-beam-epitaxy (MBE) technique is reported to possess a record high ZT $\approx$ 2.4 at room temperature.[15]

Molybdenum disulfide (MoS$_2$), a transition metal dichalcogenide, is found to be another potential material for application.[16] The properties of MoS$_2$ vary with the thickness due to its unique layer thickness-dependent electrical properties. Recent studies predict that a favorable density of state and electronic properties of MoS$_2$ may also result in an enhanced Seebeck effect, different from graphene.[17,18] Theoretical studies of MoS$_2$ nanoribbons have predicted a high ZT value (=3.0) at room temperature due to lower value of thermal conductivity and higher value of electrical conductivity. A high Seebeck coefficient value (600 $\mu$V K$^{-1}$) has been reported in the bulk MoS$_2$,[19] although its poor electrical conductivity impedes the performance in intrinsic MoS$_2$. With Bi$_2$Te$_3$ and Sb$_2$Te$_3$ being excellent materials at room temperature due to their high electrical conductivity and low thermal conductivity values,[15,20] using multilayer structures of these materials with MoS$_2$ layers offers attractive prospects.

In the present study, we aim to realize a synergic combination of properties of MoS$_2$ and Sb$_2$Te$_3$ in Sb$_2$Te$_3$/MoS$_2$ multilayered heterostructure grown by a low-cost and simple method of physical layer deposition – magnetron sputtering. Such structures are expected to offer suitable phonon and electron transport properties for the enhanced Seebeck coefficient and reduced thermal conductivity values. The influence of multiple Sb$_2$Te$_3$/MoS$_2$ interfaces on the electrical and thermal properties in Sb$_2$Te$_3$/MoS$_2$ multilayers is investigated in detail.

In order to quantify the TE performance of this advanced composite material, the present work introduces a novel method of measuring anisotropic thermal transport in complex materials nanostructures, the property pivotal in numerous applications and that is also extremely difficult to quantify. To understand and determine the values of thermal conductivity, Parker’s laser flash method, Cowan’s modified flash method, photothermal methods, Angstrom, and modified Angstrom method have been widely reported in the literature.[21–24] Most of these methods are based on the optical flash approach and are generally limited to the case of bulk materials, with thicknesses greater than 100 $\mu$m and incapable of measuring in-plane thermal conductivities. 3ω method, based on the electro-thermal heating combined with an analytical model allows to determine the thermal conductivity of the bulk as well as thin film samples with thicknesses larger than 200 nm in a simple and accurate manner.[25] However, it lacks capability to measure materials and structures involving nano-objects, multi-layers, and complex nanoscale geometries, where space constraints do not allow to perform the measurements in the preferred configuration.[26–28] Furthermore, as reported by Jaber et al.,[29] the validity of the original 3ω method using analytical models that consider infinite media and translational invariance, is limited in low-dimensional materials and systems.

Therefore, in the case of the material systems we are reporting here, that involve multiple nanoscale layers of two completely different material systems, with different mean free paths and anisotropy ratios, and for similar structures, it becomes pertinent to apply appropriate methods capable of quantitative estimation of anisotropic thermal conductivity in the nanoscale regime. This becomes essential in the development of complex nanostructured materials systems based on 2D materials that offer numerous practical applications based on size effects. In this view, scanning thermal microscopy (SThM), a modality of a scanning probe microscopy provides the required lateral resolution along with its unique ability to quantify nanoscale variations in the thermal conductivity and temperature across a sample. Unfortunately, as the nature of the tip-surface contact and interlayer contact resistance varies strongly in multi-interfaced materials, it is difficult to quantify the values of thermal conductivity with conventional SThM methods.[29–32] Moreover, the scanning probe techniques commonly used are restricted to surfaces and are incapable of approaching the thermal transport in buried and underlying structures. In this study, we advance this approach by using novel cross-sectional SThM (xSThM) that utilizes a simple sample preparation technique using Ar-ion-based beam exit cross-sectional polishing (BEXP) along with SThM to quantify thermal conductance in complex multilayer nanostructures and to measure local thermal conductivity.[15] The combined tool creates close to the atomically flat section of varied thickness which is easily accessible further, enabling the SThM analysis of the subsurface layers. Furthermore, as the dependence of the thermal transport on layer thickness is modified by the anisotropy of the thermal conductivity, we use an analytical Muzychka–Spièce model,[33,34] to independently quantify the absolute values of in-plane ($k_{xx}$) and out-of-plane ($k_{zz}$) thermal conductivities. This approach also eliminates the effect of variation of tip surface contact and interlayer contact resistance, making the present method the most reliable and versatile. As a matter of fact, the ease of this approach and the extreme sensitivity to local physical properties, initially adopted by Spièce et al. for larger systems[35] make the present technique most flexible in terms of the thickness of samples and complexity of the structures.

2. Results and Discussions
The pristine Sb$_2$Te$_3$ and multilayer Sb$_2$Te$_3$/MoS$_2$ samples prepared as described in the experimental section, were measured via X-ray diffractometry (XRD) (Figure 1). XRD peaks of the Sb$_2$Te$_3$ thin film sample reveal the growth of the rhombohedral Sb$_2$Te$_3$ phase (JCPDS- 15–0863) with the highest intensity peak corresponding to (015) plane observed at 28.8.$^\circ$[36] All the observed diffraction peaks in the multilayer samples are similar to those observed in the Sb$_2$Te$_3$ thin film sample. The orientation of the Sb$_2$Te$_3$ in multilayer samples is different from the pristine Sb$_2$Te$_3$ thin film sample. The peak corresponding to (006) plane has the highest intensity in the multilayer sample, while the peak corresponding to (015) has the highest intensity in the Sb$_2$Te$_3$ thin film sample.
These results indicate that Sb$_2$Te$_3$ thin film grows preferably along (001) direction in multilayer samples, while the pristine Sb$_2$Te$_3$ thin film has polycrystalline nature with a lower degree of preferred orientation. No MoS$_2$ peaks were observed, and also there was no shift in the position of Sb$_2$Te$_3$ peaks in the multilayer samples due to the lower thickness of the MoS$_2$ film. The strong and sharp XRD peaks observed from the all-prepared sample indicate a high degree of crystallinity.

To confirm the presence of the MoS$_2$ phase in the multilayer thin film samples, Raman measurement was carried out at room temperature with a 514 nm wavelength laser. Three Raman active modes were observed in Sb$_2$Te$_3$ thin film sample, as shown in Figure 1b. The three modes correspond to $A_g$ at 68 cm$^{-1}$, $E_g$ at 114 cm$^{-1}$ and $A_2g$ at 162 cm$^{-1}$, where the other peaks may be representing Te–Te interaction or surface oxide in the thin film sample.[36,37] The Raman spectrum of MoS$_2$ has two prominent Raman active mode; one corresponds to the in-plane ($E_g$) mode (at 383 cm$^{-1}$) and other corresponds to the out-of-plane ($A_{1g}$) mode (at 407 cm$^{-1}$).[38–40] In the in-plane mode, sulfur (S) atoms vibrate in one direction and molybdenum (Mo) atoms in the opposite direction, while in the out-of-plane mode, sulfur atoms vibrate out of the plane of MoS$_2$.[41–44] The difference in the position of the two modes increases with the number of layers of MoS$_2$ as it goes from monolayer to bulk.[45,46] In the multilayer sample, five peaks were observed in the Raman spectra. Three peaks corresponding to Sb$_2$Te$_3$ phase are observed as described above, and an additional two peaks observed in the Raman spectra indicate the presence of MoS$_2$ in the multilayer samples. MoS$_2$ peaks observed at 383 cm$^{-1}$ and 411 cm$^{-1}$ correspond to $E_g$ and $A_{1g}$ respectively in the both Sb$_2$Te$_3$/MoS$_2$ multilayer samples as shown in Figure 1b. The relative intensity of Sb$_2$Te$_3$ Raman peaks decreases and that of the MoS$_2$ peaks increases while going from Sb$_2$Te$_3$/M5 to Sb$_2$Te$_3$/M10 sample (Figure 1c). The difference between the two prominent Raman modes corresponding to MoS$_2$ layers in both multilayer samples is ≈28 cm$^{-1}$, which indicate that the thickness of MoS$_2$ is more than 7–8 monolayers or close to the bulk value.[47]

Figure 2 shows the topographical features and the grain size in Sb$_2$Te$_3$ and Sb$_2$Te$_3$/MoS$_2$ multilayer samples as obtained from FESEM and AFM techniques. The surface topography images indicate that surface features have different morphology in Sb$_2$Te$_3$ thin film and Sb$_2$Te$_3$/MoS$_2$ multilayer samples. Sb$_2$Te$_3$ thin film sample contains a large-sized hexagonal nanocrystalline feature, as shown in Figure 2a. The morphology of the top surface consisting of Sb$_2$Te$_3$ layer seems to have been significantly modified by the introduction of MoS$_2$ layers in multilayer samples. The Sb$_2$Te$_3$/M5 multilayer sample seems to be composed of small and thin Sb$_2$Te$_3$ nanosheets with a relatively smooth surface, whereas in the case of...
Sb$_2$Te$_3$/M10 sample, a slight change in surface morphology is observed, indicating a reduction in crystallite size, as shown in Figure 2b,c. From the FESEM micrographs, it is observed that the average crystallite size is in the range of 200–300 nm in Sb$_2$Te$_3$ thin film sample, and 100–120 nm and 40–60 nm in the case of Sb$_2$Te$_3$/M5 and Sb$_2$Te$_3$/M10 multilayer samples, respectively. The surface morphology seems to become smoother upon the incorporation of the MoS$_2$ layers. The change in the Sb$_2$Te$_3$ crystallite size of multilayer thin film samples is due to lower thickness of Sb$_2$Te$_3$ thin film and lattice mismatch of the MoS$_2$ and Sb$_2$Te$_3$. This reduction in the crystallite size upon the incorporation of MoS$_2$ layers may have a profound effect on the Seebeck coefficient and thermal conductivity values.\(^{[48,49]}\)

To further confirm the roughness and the surface morphology, atomic force microscopy measurements were carried out. The average surface roughness was observed to be 10 nm in the Sb$_2$Te$_3$ thin film sample, while Sb$_2$Te$_3$/M5 and Sb$_2$Te$_3$/M10 multilayer samples manifest a decreased surface roughness value of 3 and 5 nm, respectively. The nature of the interface was analyzed by a combination of cross-sectional high-resolution TEM measurement and FESEM and are shown in Figure 3. HRTEM micrograph of the cross-section of Sb$_2$Te$_3$/M10 sample revealed distinct MoS$_2$ layers of thickness 10 nm separated by 20 nm Sb$_2$Te$_3$ layers, which is also consistent with the result of FESEM measurement shown in Figure 3d.

The dark and bright strip corresponds to MoS$_2$ and Sb$_2$Te$_3$ layers, respectively, and are observed with the contrast arising due to atomic mass difference. The observed fringe pattern corresponding to Sb$_2$Te$_3$ layer indicates the crystalline phase with interplanar distance 1 nm, whereas the absence of clear fringes in the MoS$_2$ layers indicates it to be comprised of isolated MoS$_2$ domains with relatively poor overall crystallinity. These results justify the XRD spectra, where no MoS$_2$ diffraction patterns were observed.

To understand the charge transport behavior at the MoS$_2$ and Sb$_2$Te$_3$ interface, Hall measurements were carried out at room temperature. The values of carrier concentration, Hall mobility, electrical conductivity, Seebeck coefficient, and power factor are given in Table 1. The carrier concentration values decreased as MoS$_2$ layers were incorporated into the multilayer samples. However, the value of Hall mobility was observed to increase in the case of Sb$_2$Te$_3$/MoS$_2$ multilayer samples. It was observed that the Sb$_2$Te$_3$/MoS$_2$ multilayer sample exhibits considerably higher mobility (59.49 ± 3 cm$^{-1}$ s$^{-1}$) and lower carrier concentration ((1.9 ± 0.08) × 10$^{19}$ cm$^{-3}$) as compared to Sb$_2$Te$_3$ sample (35.16 ± 2 cm$^{-1}$ s$^{-1}$ and 13.5 ± 0.7 × 10$^{19}$ cm$^{-3}$, respectively) at 316 K. The enhancement in the carrier mobility value of Sb$_2$Te$_3$/MoS$_2$ multilayer samples is due to preferred orientation [001] growth and high mobility of MoS$_2$, which provide a relatively preferential route for the charge carrier transport. Moreover, according to the previous reports on the similar topological insulator, Bi$_2$Te$_3$, with high mobility surface states, the mobility is increased for the lower thicknesses\(^{[28,50]}\) suggesting a similar behavior of Sb$_2$Te$_3$ that is also a good topological insulator material. As a matter of fact, for enhanced ZT values, the combination of S and $\sigma$ needs to be elevated.\(^{[51,52]}\) It is well known that for a degenerate semiconductor, S is inversely proportional to carrier concentration and directly proportional to mobility of carriers.\(^{[53,54]}\) Whereas, $\sigma$, is directly proportional to both carrier concentrations and carrier mobility. Therefore, an enhanced mobility and optimized carrier concentration ($\approx$10$^{18}$–10$^{19}$ cm$^{-3}$), in the case of degenerate semiconductors, are the keys for high power factors.\(^{[55,56]}\) In the case of Sb$_2$Te$_3$/MoS$_2$ samples better TE properties can be expected as it demonstrates higher mobility (58.16 ± 2.8 cm$^{-1}$ s$^{-1}$) and optimized ranges of carrier concentration ($\approx$1.9 × 10$^{19}$ cm$^{-3}$) as compared to Sb$_2$Te$_3$ thin film.

Figure 4 shows the results of the electrical conductivity and the Seebeck coefficient measurements in the in-plane direction for the Sb$_2$Te$_3$ and Sb$_2$Te$_3$/MoS$_2$ multilayer samples in the temperature range from 320 to 484 K. The temperature

Table 1. The carrier concentration, electrical conductivity, Seebeck coefficient, Hall mobility and power factor values of Sb$_2$Te$_3$ and Sb$_2$Te$_3$/MoS$_2$ samples at 316 K.

| Sample name       | Carrier concentration 10$^{19}$ [cm$^{-3}$] | Electrical conductivity [Scm$^{-1}$] | Hall mobility [cm$^2$ V$^{-1}$ s$^{-1}$] | Seebeck coefficient [$\mu$VK$^{-1}$] | Power factor [mWm$^{-1}$ K$^{-2}$] |
|-------------------|---------------------------------------------|------------------------------------|------------------------------------------|--------------------------------------|-----------------------------------|
| Sb$_2$Te$_3$      | 13.5 ± 0.7                                  | 597 ± 29                           | 27 ± 1                                   | 188 ± 9                              | 2.1 ± 0.2                         |
| MoS$_2$           | 0.52 ± 0.03                                 | 5.5 ± 0.3                          | 11.2 ± 0.6                               | –706.4$^{[44]}$                      | -                                 |
| Sb$_2$Te$_3$/M5   | 4.8 ± 0.1                                   | 356 ± 17                           | 46 ± 2                                   | 286 ± 14                             | 2.9 ± 0.2                         |
| Sb$_2$Te$_3$/M10  | 1.9 ± 0.08                                  | 176 ± 8                            | 58 ± 3                                   | 530 ± 26                             | 4.9 ± 0.4                         |
dependence of electrical conductivity in \( \text{Sb}_2\text{Te}_3 \) and \( \text{Sb}_2\text{Te}_3/\text{MoS}_2 \) multilayer thin film samples are different, as shown in Figure 4a. In \( \text{Sb}_2\text{Te}_3 \) thin film, the electrical conductivity values increase with an increase in the temperature from 320–400K, indicating semiconducting behavior,[57] and beyond 400 K, the electrical conductivity value was observed to get saturated and remained such from 400–484 K. However, the change in the electrical conductivity values as a function of temperatures for \( \text{Sb}_2\text{Te}_3/\text{MoS}_2 \) multilayer samples is negligible as compared to the pristine \( \text{Sb}_2\text{Te}_3 \) thin film sample.

The value of electrical conductivity for \( \text{Sb}_2\text{Te}_3 \) thin film sample (597 ± 29 S cm\(^{-1}\) at 316 K) is higher than the \( \text{Sb}_2\text{Te}_3/\text{M}5 \) (356 ± 17 S cm\(^{-1}\) at 316 K) and \( \text{Sb}_2\text{Te}_3/\text{M}10 \) (176 ± 8 S cm\(^{-1}\) at 316 K). It is evident that the introduction of \( \text{MoS}_2 \) thin layer in \( \text{Sb}_2\text{Te}_3 \) thin film reduced the electrical conductivity values and further increase in the \( \text{MoS}_2 \) thin film thickness in \( \text{Sb}_2\text{Te}_3/\text{M}10 \) sample, results in further reduction in the value of electrical conductivity. It is clearly evident from Hall measurements that with the increase in \( \text{MoS}_2 \) thickness in the multilayer samples, the carrier concentration was observed to decrease. The reduction in the electrical conductivity values in \( \text{MoS}_2/\text{Sb}_2\text{Te}_3 \) multilayer samples is due to the reduced carrier concentration.[58] Since \( \text{Sb}_2\text{Te}_3/\text{MoS}_2 \) multilayer samples possess much smaller grains size as compared to the pristine \( \text{Sb}_2\text{Te}_3 \) thin film, the possibility of a decline in electrical conductivity due to a reduction in grain size cannot be ruled out.[59,60]

The Seebeck coefficient of \( \text{Sb}_2\text{Te}_3 \) and \( \text{Sb}_2\text{Te}_3/\text{MoS}_2 \) multilayers thin film samples exhibit positive values, revealing p-type semiconducting behavior within the temperature range of 320–484 K, as shown in Figure 4b. Higher Seebeck coefficient values were observed in both the multilayer \( \text{Sb}_2\text{Te}_3/\text{MoS}_2 \) samples as compared to the pristine \( \text{Sb}_2\text{Te}_3 \) thin film sample. The enhancement in the Seebeck coefficient values in multilayer samples is an important result of the present study and will be discussed later in detail. The Seebeck coefficient in the pristine \( \text{Sb}_2\text{Te}_3 \) thin film sample increases with an increase in temperature up to 450 K and seems to reach its saturation after that. However, in \( \text{Sb}_2\text{Te}_3/\text{M}5 \) multilayer sample, the Seebeck coefficient values increase with an increase in the temperature up to 433 K and then start decreasing, whereas the Seebeck coefficient value in \( \text{Sb}_2\text{Te}_3/\text{M}10 \) multilayer sample increases with an increase in temperature up to 347 K and after that tends to decrease relatively faster. This reduction in the Seebeck coefficient with elevated temperature may be due to the increased contribution of minority carriers (i.e., electrons).[61,62]

It is very well known that the \( \text{Sb}_2\text{Te}_3 \) is p-type, and \( \text{MoS}_2 \) is an n-type semiconductor material. Therefore, at a high temperature, holes from \( \text{Sb}_2\text{Te}_3 \) and electrons from \( \text{MoS}_2 \) contribute to the total Seebeck coefficient value of \( \text{Sb}_2\text{Te}_3/\text{MoS}_2 \) multilayer samples. The average weighted Seebeck coefficient is expressed as\(^{[3]}\)

\[
S = \frac{S_p \sigma_p + S_n \sigma_n}{\sigma_p + \sigma_n}
\]

where \( S \) is the measured Seebeck coefficient, \( \sigma \) is the electrical conductivity, and \( p \) and \( n \) indicate hole and electron-related transport processes. Since the two charge carriers with opposite signs contribute to the Seebeck coefficients, the resultant...
Seebeck coefficient reduces at increased temperatures due to bipolar thermo-diffusion. A higher value of the Seebeck coefficient (530 ± 26 µV K⁻¹) is observed in Sb₂Te₃/M10 sample at 316 K, which is almost three times (188 ± 9 µV K⁻¹) higher in comparison to that observed in Sb₂Te₃ thin film sample. The schematic illustration showing the effect of the interface on the charge carrier in the Sb₂Te₃/MoS₂ multilayer samples is shown in Figure 4c. The potential barrier is produced at the interface due to a difference in the work function value of Sb₂Te₃ and MoS₂. The energy band diagram is based on work function values for Sb₂Te₃ (4.6 eV), and MoS₂ (5.2) measured by Kelvin probe force microscopy, see the supporting information (Supporting Information, S2). The measured work function value of Sb₂Te₃ and MoS₂ matches well with the previously reported values. Our previous study on the nature of interface at various MoS₂ thicknesses showed the presence of excess charge accumulated in the MoS₂ layer due to its low thickness, and this excess charge layer will act as a potential barrier for the majority charge carrier holes. This potential barrier restricts the low-energy holes at the interface resulting in carrier filtering effect. In carrier filtering effects, the lower energy carriers (holes) are scattered or blocked by the hetero-interface, and the relative contribution of lower energy carriers is reduced in comparison to higher energy carriers resulting in enhanced Seebeck coefficient values. The presence of a potential barrier at the interface, also explains the lower values of electrical conductivity in the case of Sb₂Te₃/MoS₂ multilayer sample due to the scattering of the lower energy holes at the interface. Additionally, the enhancement of the Seebeck coefficient value in the Sb₂Te₃/M10 is also due to a large Seebeck coefficient value of MoS₂.

The calculated power factor (S²σ) values for Sb₂Te₃ and Sb₂Te₃/MoS₂ multilayer samples are shown in Figure 4d. Although the electrical conductivity exhibits a lower value in multilayer samples, the increase in the Seebeck coefficient is significantly higher, and this trade-off between σ and S, results in an enhanced value of power factor in the multilayer samples. A high value of power factor 4.9 ± 0.4 x 10⁻³ Wm⁻¹ K⁻² was observed at 316 K in the Sb₂Te₃/M10 multilayer sample, which is ~2.5 times higher than that observed in Sb₂Te₃ thin film sample (2.1 ± 0.2 x 10⁻³ Wm⁻¹ K⁻²). We believe that the clearly observed enhancement in the Seebeck coefficient values of Sb₂Te₃/M10 samples with numerous thin layers (20 nm/10 nm) is due to the carrier filtering effect. Furthermore, the Sb₂Te₃/M10 multilayer thin film sample has a higher carrier mobility as compared to the Sb₂Te₃ thin film due to its preferred orientation growth. The preferred orientation plane establishes a reasonably favored mode for charge carrier transport and increase the charge carrier mobility. It plays a significant role in enhancing the power factors of the Sb₂Te₃/M10 multilayer thin film samples.

To understand the thermal transport of multilayer samples and its effect on thermoelectric properties, it is necessary to look at the in-plane thermal conductivity values. Therefore, to simultaneously measure the in-plane and out-of-plane values of thermal conductivity a novel technique of xSThM has been used (see Experimental Section). In order to eliminate the material – dependent tip-surface thermal resistance in the case of multilayer sample, the xSThM measurements use low angle BEXP cut samples. As the heat spreading in the layered sample on a substrate is directly affected by the anisotropy of its thermal conductivity, by fitting the xSThM measured dependence of the thermal resistance on the wedge thickness, t, in the point of contact via analytical Muzychka–Spieč model, we will obtain both the in-plane (κxy) and out-of-plane (κz) values of thermal conductivity. The total thermal resistance measured, Rx(t) is a sum of the constant thermal resistance of the probe-sample contact, RC, and the spreading thermal resistance, Rx(t):

\[
R_x(t) = R_x(1) + R_C
\]

While it is possible in principle to also independently evaluate the contribution of interfacial (layer-substrate) thermal resistivity, rint, as well, we show (Supporting Information, S3.3.2) that for the range of thermal conductivities typical for our samples and within a broad range of possible rint reported elsewhere, rint does not affect the measured xSThM dependences and therefore does not affect the derived κxy and κz values.

The model we use here uses the fact that the mean free path in Sb₂Te₃ is on the order of a few nm and much smaller than the dimensions of the contact (defined by the tip apex dimensions of a few tens of nm) and thickness of the layer used for the fitting (from tens to hundreds of nm) making a diffusion approximation a viable approach.

For xSThM measurements, a layer of TE material (e.g., Sb₂Te₃/MoS₂) deposited on the 300 nm SiO₂ layer thermally grown on thick (400 µm) Si substrate is cut by the BEXP producing extremely smooth (few nm roughness) cut across all layers as shown in topography (Figure 5a,b). A SThM data are simultaneously acquired (Figure 5c, d) producing the data of Rc(t). The whole measurement cycle, therefore, takes less than a few minutes. The processing of the data consists of two steps. First, a SiO₂ layer that has a known thermal conductivity, is used to evaluate the contact radius of the tip-surface contact, a, and the dimensionless SThM probe constant, cₓ, the ratio of the probe response to the self-heating and heat transferred to the sample. Parameter a is essential for determining the anisotropy of the heat conductance, whereas cₓ is required for the quantitative measurements of the thermal conductivity. These two parameters are determined in a single fit of the nonlinear dependence of Rx(t) for SiO₂ layer on Si versus analytical isotropic model described in detail below. By using the difference of the thermal resistance for thickness t and thickness t = 0, such as Rx(t) - Rx(0), we eliminate the generally unknown tip-sample thermal resistance. In the second step, the obtained a and cₓ values obtained previously are used for fitting values of κxy and κz of the layer of interest versus analytical anisotropic model below. At each only two parameters of a single curve are to be fitted producing high-quality reliable measurement results.

In xSThM measurement, we can consider each point of measurement of Rx on the wedge cut sample as measurement on a layer of variable thickness. Therefore, each data point can be treated as a material having value of thermal conductivity κm on the substrate having value of thermal conductivity κs. For the isotropic sample, such as SiO₂ layer on Si, we use an
isotropic model for calculating spreading resistance $R_s$ as a function of thickness given as $[33,34]$

$$R_s(t) = \frac{1}{\pi \kappa_m a_0} \left[ \frac{1 + K \exp\left( -\frac{2\xi t + a}{a} \right)}{1 - K \exp\left( -\frac{2\xi t + a}{a} \right)} \right] J_1(\xi) \sin(\xi) \frac{d\xi}{\xi}$$  \hspace{1cm} (3)

where $a$ is the radius of the tip, $r_{\text{int}}$ is the interfacial thermal resistance per unit area, $t$ is the thickness of the layer, $\kappa$ is the integration variable, $J_1$ is the first order Bessel function and

$$K = \frac{1 - \left( \frac{\kappa_x}{\kappa_m} \right)^2}{1 + \left( \frac{\kappa_x}{\kappa_m} \right)^2}$$  \hspace{1cm} (4)

From the experiment, we are measuring $R_x$ so Equation (2) can be rewritten as

$$R_x(t) - R_s = R_c(t)$$  \hspace{1cm} (5)

The absolute values of contact thermal resistances are obtained by determining the probe to base thermal resistance

$$c_a \cdot [R_x(t) - R_s(0)] = \left[ \frac{1}{\pi \kappa_m a_0} \left[ \frac{1 + K \exp\left( -\frac{2\xi t + a}{a} \right)}{1 - K \exp\left( -\frac{2\xi t + a}{a} \right)} \right] J_1(\xi) \sin(\xi) \frac{d\xi}{\xi} \right]$$

$$= \left[ \frac{1}{\pi \kappa_m a_0} \left[ \frac{1 + K \exp\left( -\frac{2\xi t + a}{a} \right)}{1 - K \exp\left( -\frac{2\xi t + a}{a} \right)} \right] J_1(\xi) \sin(\xi) \frac{d\xi}{\xi} \right]$$  \hspace{1cm} (6)

where $a$ is the anisotropy ratio $a = k_{xy}/k_z$.

Thereafter, Equation (7) has been used for fitting of the experimental data for SiO$_2$/Si interface to extract the values of $a$ and $c_a$ (see also Supporting Information, S3.3.2). The values of $a$ and $c_a$ were used in the anisotropic model for thermally anisotropic material to quantify the value of $k_{xy}$ and $k_z$. For the anisotropic model the values of $a$ and $\kappa_m$ are replaced by

$$t = \sqrt{\kappa_x \kappa_y}$$  \hspace{1cm} (8)

$$\kappa_m = \sqrt{k_x k_y}$$  \hspace{1cm} (9)

where $a$ that links the power applied to the SThM probe heater and the average temperature rise of the heater due to self-heating as described in detail. The probe-sample thermal resistance, $R_s$, is different from $R_x$ by a multiplication factor, $c_a$, that is the ratio of the change in the average probe temperature (the value measured in SThM) due to self-heating to the change of the average probe temperature due to the same amount of heat lost to the sample via probe apex. This multiplication factor is the unique value for each SThM probe and being a ratio, does not depend on the power applied to the probe as described in details elsewhere.

Further, to eliminate unknown parameter ($R_s$), for the ease of fitting, Equation (5) can be expressed as

$$c_a \cdot [R_x(t) - R_s(0)] = R_x(t) - R_s(0)$$  \hspace{1cm} (6)

It is essential as we mentioned above, that one of the benefits of BEXP nano-polishing process is that it produces an extremely smooth and minimally damaged surface allowing to assume $R_s$ independent of thickness.

Substituting the values of $R_s(t)$ and $R_s(0)$ from Equation (3) in Equation (6) we get

$$c_a \cdot [R_x(t) - R_s(0)] = \left[ \frac{1}{\pi \kappa_m a_0} \left[ \frac{1 + K \exp\left( -\frac{2\xi t + a}{a} \right)}{1 - K \exp\left( -\frac{2\xi t + a}{a} \right)} \right] J_1(\xi) \sin(\xi) \frac{d\xi}{\xi} \right]$$  \hspace{1cm} (7)
Information. The value of thermal resistance as a function of thickness has been evaluated using below formula

\[
R_x = \frac{V_{nc}R_x}{V_{nc} - V_{Th}} \quad (10)
\]

where \(V_{nc}\) is the voltage of the probe when tip is not in contact with any surface, \(R_p\) is the thermal resistance of the probe and \(V_{Th}\) is the thermal voltage of the tip in contact with the sample surface. The experimental values of \(R_x\) versus thickness for Si/SiO2 interface were plotted along with the simulated curves (curves plotted using Equation 7), by fixing the values of \(a\), \(r_{int}\), \(e\), \(κ_m\), and \(κ_s\), to determine the general ranges of unknown \((a, r_{int}\) and \(e)) and has been discussed in detail in Supplementary Information (S3.3.2). The experimental curves for Si/SiO2 interface were then fitted in Muzychka–Spiece model (Equation 7) to determine the values of \(a\), \(r_{int}\), and \(e\), and are tabulated in Table 2.

The values of thermal conductivity for Si and SiO2 were assumed to be 130 ± 5 Wm\(^{-1}\)K\(^{-1}\) and 1.4 ± 0.1 Wm\(^{-1}\)K\(^{-1}\) respectively.\(^{[78,79]}\) There are several reports, citing values of thermal conductivity for amorphous SiO2 between 1.0–1.4 Wm\(^{-1}\)K\(^{-1}\)\(^{[78,80,81]}\) depending on the growth mechanism and layer thickness. At the same time, given the phonons mean free path in the amorphous SiO2 on the 10 nm length scale, consistent with reports by Cahill et. al. and Braun et. al. reporting no substantial change in the value of thermal conductivity of SiO2 for film thickness above 100 nm\(^{[82,83]}\) we use the widely reported value of 1.4 ± 0.2 Wm\(^{-1}\)K\(^{-1}\). It is to be noted that this provide the conservative estimate for the thermal conductivity of Sb2Te3/MoS2 and the claimed higher ZT value.

\(R_x\) as a function of thickness for Sb2Te3, Sb2Te3/M5, and Sb2Te3/M10 samples were plotted and are shown in Figure 6. Along with the experimental data for \(R_x\) versus thickness, simulated curves evaluated using Equation 7 (anisotropic model), were also plotted. The values of \(a\), and \(e\) were then used to determine the values of \(κ_{xy}\) and \(κ_s\) for Sb2Te3, Sb2Te3/M5, and Sb2Te3/M10 (Table 2). Results from fitting clearly indicate a lower value of thermal conductivity for the multilayer samples (Sb2Te3/M5 and Sb2Te3/M10) as compared to the pristine sample both in the in-plane and out-of-plane directions shown in Figure 7.

It can be observed from the figure that the materials having higher direction averaged thermal conductivity \(κ_m = \sqrt{κ_{xy}κ_z}\) than the substrate (\(κ_m > 1.4\) Wm\(^{-1}\)K\(^{-1}\)) show negative slope of \(R_x\) as a function of thickness. Therefore, it can be inferred from the comparison of the experimental data and the simulated curves that the direction averaged thermal conductivity for pristine Sb2Te3, \(κ_m\), is between the thermal conductivity of the substrate SiO2 (1.4 Wm\(^{-1}\)K\(^{-1}\)) and 3 Wm\(^{-1}\)K\(^{-1}\), that fits well with the 3ω measurements (for \(k_{SiO2}=1.52\) Wm\(^{-1}\)K\(^{-1}\) and \(k_{SiO2}=4.5\) Wm\(^{-1}\)K\(^{-1}\)) \(^{[84–74]}\) It is worth noting here that, unlike Sb2Te3/M5 and Sb2Te3/M10 samples, assumptions and boundary conditions of 2D analytical model (invariance in z-direction and thickness of layer > 200 nm) still holds for Sb2Te3 sample making the value of thermal conductivity in the case of Sb2Te3 sample, having thickness >250–300 nm, obtained through 3ω method (described in detail in Supporting Information), is in reasonable accordance with the xSThM values and values reported in the literature. Due to unreliable thermal transport data and poor fitting, the exact values of thermal conductivity and anisotropy ratios \((a)\) for pristine Sb2Te3 were not determined (consequently, ZT for Sb2Te3 has been calculated taking the value of thermal conductivity obtained from 3ω method). At the same time, one can see that the value of thermal conductivity for multilayer samples (Sb2Te3/M5 and Sb2Te3/M10) clearly lies in between the range of 0.5-1.0 Wm\(^{-1}\)K\(^{-1}\). It is clear that the above assumptions (large thickness, uniformity, etc.) in the case of multi-layer samples (Sb2Te3/M5 and Sb2Te3/M10 samples) are not valid, and one cannot use the values of thermal conductivity of the nanolayers obtained via 3ω with xSThM is being much better technique applicable in the case of multi-layered and complex structures. Also, it should be noted that xSThM is best used for the values of the thermal conductivity of the probed layer placed on the higher thermal conductivity substrate – that is exactly the case for the Sb2Te3/M5 and Sb2Te3/M10 on the SiO2 layer. It can be clearly seen from Table 2, that the thickness of MoS2 also has

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**Table 2.** The values of \(a\), \(r_{int}\), \(κ_m\) for SiO2/Si interface and \(r_{int}\), \(κ_{xy}\) and \(κ_s\) for sample/SiO2 interface. (Units of \(κ_{xy}\), \(κ_s\), \(κ_{xy}/\kappa_z\) and \(κ_z\) are in \(\text{Wm}^{-1}\text{K}^{-1}\)).

| Sample name                    | \(Si_\text{SiO2}\) | \(a (\text{nm})\) | \(c_s\) | \(r_{int} \times 10^9 \text{[Km}^2\text{W}^{-1}]\) | \(r_{int} (10^9)\) | \(κ_m\) | \(κ_{xy}\) | \(κ_s\) | \(κ_{xy}/\kappa_z\) | \(κ_s\) | \(κ_z\) | \(ZT\) |
|-------------------------------|---------------------|---------------------|----------|------------------------------------------------|---------------------|---------|-----------|---------|----------------------|---------|---------|--------|
| Sb2Te3                        |                     | 39                  | 8.41     | 0.01                                             | –                   | >1.4    | 0.9 ± 0.1 | 0.5 ± 0.1 | 1.5 ± 0.2                  | 0.28    | 0.62    | 0.96 ± 0.26 |
| Sb2Te3/M5                     |                     | 35                  | 6.63     | 4.80                                             | 10.9                | 0.7 ± 0.1 | 0.6 ± 0.1 | 1.1 ± 0.2 | 0.14                               | 0.14    | 0.58    | 2.08 ± 0.37 |
| Sb2Te3/M10                    |                     | 35                  | 5.74     | 9.83                                             | 10.3                | 0.6 ± 0.1 | 0.6 ± 0.1 | 1.1 ± 0.2 | 0.14                               | 0.14    | 0.58    | 2.08 ± 0.37 |

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**Figure 6.** Thermal resistance as a function of thickness of Sb2Te3, Sb2Te3/M5 and Sb2Te3/M10 samples. Curves with lines + symbol are showing the experimental data and curves with symbol are showing simulated curves plotted using Equation 7 with fixed \(a\) and \(r_{int}\) (from the respective Si/SiO2 interface fitting analysis) and varying values of \(κ_m\) and anisotropy ratio \((a) = κ_{xy}/κ_z\).
an effect on the anisotropy ratios of thermal conductivity, and as the thickness of MoS$_2$ increases in multi-layered structure the anisotropy ratio was observed to decrease. Therefore, it was observed that although Sb$_2$Te$_3$ might have increased anisotropy in multi-layered structures, the multilayer material as a whole offer lower anisotropy than the pristine Sb$_2$Te$_3$, with the value of anisotropy ratios ($a_r = \frac{k_{xy}}{k_z}$), depending on the thickness of MoS$_2$ layers as well.

Additionally, it can be observed from Figure 6 that both the multilayer samples show oscillations in the region of the multilayer. This can be attributed to the difference in the values of thermal conductivity of individual layers of Sb$_2$Te$_3$ and MoS$_2$ and possibly to the variation of the interfacial thermal resistance between the SiO$_2$/multilayer sample and between Sb$_2$Te$_3$/MoS$_2$ layers. However, as the ZT is determined by the overall thermal conductivity of multilayer samples in the in-plane direction, the average of these oscillations can be fitted in the Muzychka–Spiece model.[33,34] Therefore, despite of the modulation present in the experiment data, due to multiple interfaces in the case of multilayer samples, the average of the oscillations after fitting, gave reliable value of the thermal conductivity in the in-plane and out of the plane direction. The total thermal conductivity value is the contribution of electronic ($\kappa_e$) and lattice ($\kappa_l$) thermal conductivity. The electronic thermal conductivity of all the samples were obtained by using Wideman-Franz relation ($\kappa_e = \sigma L T$), where $T$ is the temperature and $L$ is the Lorentz number. Compared to the multi-layered samples, pristine Sb$_2$Te$_3$ exhibits a higher value of electronic thermal conductivity, which is due to the enhancement in the values of electrical conductivity. The lattice thermal conductivity of all the samples were calculated using equation $\kappa_l = \kappa - \kappa_e$. The value of the lattice thermal conductivity was observed to decrease with increase in the MoS$_2$ film thickness in the multilayer samples as shown in Table 2. The reduction of the lattice thermal conductivity value can be attributed due to the large phonon scattering at interface or lower values of thermal conductivity of MoS$_2$. Various phonon scattering mechanisms are known to contribute to decrease the thermal conductivity such as phonon–phonon scattering (Umklapp process), phonon-grain boundary scattering, phonon-interface scattering, point defect scattering, and phonon-electron scattering.[10,55,66] In addition, there are other factors which are also responsible for reduction in the values of thermal conductivity of the materials such as phase transition, doping, and alloying.[86–88] Several theoretical reports have explained the reduction in the $\kappa$ value in the multilayer structure based on phonon interface scattering, which reduces the phonon's mean free path and group velocity.[11,89] Moreover, MoS$_2$ has low thermal conductivity values, which has further increased the interface phonon scattering.[90] These results clearly indicate lower values of thermal conductivity in the Sb$_2$Te$_3$/MoS$_2$ multilayer samples as compared to the Sb$_2$Te$_3$ thin film samples. The calculated ZT values for Sb$_2$Te$_3$ and Sb$_2$Te$_3$/MoS$_2$ multilayers samples are shown in Table 2. A high value of ZT 2.08 ± 0.37 was observed at 316 K in the Sb$_2$Te$_3$/M10 multilayer sample, which is ≈5 times higher than that observed in Sb$_2$Te$_3$ thin film sample (0.42 ± 0.07). The 2D/three-dimensional (2D/3D) interface effect plays a very crucial role in the properties of MoS$_2$/Sb$_2$Te$_3$.
multilayer thin film samples. The low-energy charge carriers from Sb$_2$Te$_3$ are scattered from the MoS$_2$ layers and only high-energy charge carriers can tunnel through the MoS$_2$ layers. The thickness of the MoS$_2$ layers is very thin which provides a channel to promote the charge carrier transport, which further results in enhanced values of the Seebeck coefficient and high mobility. In addition, lower thickness of Sb$_2$Te$_3$ layers also contributed to the enhancement in the values of power factor in the case of MoS$_2$/Sb$_2$Te$_3$ multilayer samples due to topological insulator effect.[20,50] The pristine Sb$_2$Te$_3$ thin film sample investigated in the present study has properties comparable to those reported for Sb$_2$Te$_3$ thin films.[8,18]

As mentioned earlier, different approaches such as nano-composite, doping, core—shell, and multilayer structure have been reported for improving the response of Bi$_2$Te$_3$, Sb$_2$Te$_3$, and similar compounds.[18,57,90,91] However, the present methodology of using a multilayer structure seems to be more effective as it enhances the power factor along with a simultaneous reduction in thermal conductivity values. Venkatasubramanian et. al.[15] reported the highest ZT = 2.4 at the room temperature in the p-type Bi$_2$Te$_3$/Sb$_2$Te$_3$ superlattice structure by controlling the electron and phonon transport. Tan et. al.[158] also fabricated Bi$_2$Te$_3$/ZrB$_2$ superlattice structure showing large enhancement in the power factor along with a decrease in the thermal conductivity values and ZT = 1.54 at room temperature was observed. The present results are consistent with the above reports. Here, the improvement in electron and phonon transport in multilayer samples is discussed in terms of the presence of interface barriers, as confirmed by KPFM measurements. 2D layers of MoS$_2$ and other materials having suitable thickness or number of layers may further enhance the effects mentioned here. The results of the present study give a new direction to utilize interface barriers in multilayer structures and fine-tune the electron and phonon transport for better, electrical and thermal properties, paving new pathways in the field of thermoelectric.

3. Conclusions

In this work, structural, topographical, and thermoelectric properties of the Sb$_2$Te$_3$/MoS$_2$ multilayer structure fabricated with varying thickness of MoS$_2$ layers were investigated. KPFM results show the presence of a potential barrier for majority carrier-holes, which is favorable for increased phonon scattering and energy filtering of low-energy charge carriers. The change in the crystalline orientation and grain size in Sb$_2$Te$_3$ due to MoS$_2$ incorporation and lower thermal conductivity of MoS$_2$ additionally improve electron and phonon transport. Electrical and thermal measurements revealed that Sb$_2$Te$_3$/M10 sample shows a high-power factor along with reduced thermal conductivity values in the in-plane direction as compared to the pristine Sb$_2$Te$_3$ thin film sample. The highest value of Seebeck coefficient (530 ± 26 μV K$^{-1}$ at 316 K) along with lower values of thermal conductivity (0.7 ± 0.1 W m$^{-1}$ K$^{-1}$ at RT) in the in-plane direction, observed for Sb$_2$Te$_3$/M10 multilayer samples, grown by a simple method of magnetron sputtering, are very encouraging and lead to a high value of ZT = 2.08 ± 0.37 at 316 K. The key points emerging from the present work are the direct importance of interfaces and the possibility of further improving the response of the materials by incorporating other 2D materials having layer-dependent properties for controlling the electron and phonon transport at the 2D/3D interfaces. Further, the use of combined technique of nano-cross-sectioning (BEXP with xSThM) provides a direct method of simultaneously measuring in-plane and out-of-plane thermal conductivity values of thin film which otherwise is hard to quantify.

4. Experimental Section

Sample Preparation: Sb$_2$Te$_3$/MoS$_2$ multilayer samples were deposited onto SiO$_2$/Si substrate by multilayer RF sputtering technique using 2" diameter targets of Sb$_2$Te$_3$ and MoS$_2$ with 99.9% purity via a controlled sequential deposition. Before deposition, substrates were cleaned through the RCA process to avoid contamination. The optimized values of RF power of 20 and 50 W were applied for Sb$_2$Te$_3$ and MoS$_2$, respectively, with Ar flow rate maintained at 20 sccm and substrate temperature at 150 °C during deposition time. The base pressure of the sputtering system was 5 x 10$^{-5}$ Torr, and a working pressure of 5.5 x 10$^{-3}$ Torr was used for sputtering. The targets were presputtered for 10 min to remove any contamination from the target surface. The deposition rate was 10 nm/min, and 2 nm/min for Sb$_2$Te$_3$ and MoS$_2$, respectively, which was confirmed by X-Ray reflectivity (XRR) and optical profiles (see the supplementary information, Supporting Information, S1). For the deposition of Sb$_2$Te$_3$/MoS$_2$ multilayer samples, the thickness of Sb$_2$Te$_3$ was kept fixed at 20 nm, whereas two different thickness of 5 and 10 nm were chosen for MoS$_2$. The multilayer thin film samples having MoS$_2$ modulation period 5 and 10 nm were labeled as Sb$_2$Te$_3$/M5 and Sb$_2$Te$_3$/M10, respectively. Both Sb$_2$Te$_3$/MoS$_2$ multilayer samples consist of 10 layers MoS$_2$ thin film and 11 layers Sb$_2$Te$_3$ thin film. The total thickness of the Sb$_2$Te$_3$ layers is 220 nm in all the samples, while that of MoS$_2$ layers was 50 and 100 nm making the total sample thickness to be 270 and 320 nm in Sb$_2$Te$_3$/M5 and Sb$_2$Te$_3$/M10 multilayer samples, respectively. The total thickness of Sb$_2$Te$_3$ layers has been kept constant in all the samples to evaluate the effect of MoS$_2$ layer incorporation. Particularly for thermal conductivity measurements, a novel technique of cross-sectioning the samples was employed, which allows the measurement of thermal resistance as a function of thickness.[50-72] This cross-sectioning technique uses triple Ar-ion coplanar beams which are intersecting in ~1 mm area. The beam enters the sample from its side at a small negative angle with respect to its surface (~5°). This technique is called as beam exit nano cross-section polishing (BEKP) as in a result the beam exits at a glancing angle from the surface.[70] Such polishing technique and the use of inert Ar ions offer minimum damage and near-atmospheric surface roughness (Figure 8).

Characterization Techniques: The phase and structural properties of deposited multilayer samples were investigated using an X-ray diffractometer (XRD Philips X'Pert PRO-PW 3040) with Cu Kα (λ = 1.5406 Å) radiation. The presence of Sb$_2$Te$_3$ and MoS$_2$ phases in multilayer samples were further characterized by Raman spectroscopy technique using the Horiba Scientific LabRAM HR evolution system with an argon-ion laser of 514.5 nm wavelength as the excitation source. The surface topography and microstructure of the deposited thin film samples were analyzed using a dual-beam field emission scanning electron microscope (FESEM Model Quanta 3D FEG, FEI). The cross-section investigation of Sb$_2$Te$_3$/MoS$_2$ multilayer thin film sample was carried out using a high-resolution transmission electron microscope, (HR TEM Technai G2 20 Stwin model) operating at 200 kV. Atomic force microscopy (AFM) and SThM study (Figure 8) was carried out using the Dimension Icon (Bruker). The cantilever had a radius of curvature of 30 nm and a resonance frequency of 60 kHz. The scan rate of AFM measurement was 0.7 Hz. The Seebeck coefficient and electrical conductivity nature of the samples were studied simultaneously using LSR-3 (Linseis) under controllable helium atmosphere with temperature range of 320–484 K.
Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest

The authors declare no conflict of interest.

Author Contributions

‡ MA and KA contributed equally to the work. MA, BRM, NK, AG Materials concept, sample preparation, measurements, materials characterization, methodology development and validation, data analysis of experimental data, and initial draft preparation. KA, SGM, OVK Thermal transport measurements and concepts, sample preparation, thermal transport development of the analytical model, FEA simulation, data analysis. BRM, OVK data interpretation, supervision, project and research guidance, and final manuscript preparation (All).

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords

2D/3D interfaces, energy filtering effect, phonon scattering, thermal transports, thermoelectric properties, wedge cuts, xSThM

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