Thermal transport in enhanced thermoelectric performance high FOM Sb_2Te_3/MoS_2 heterostructure

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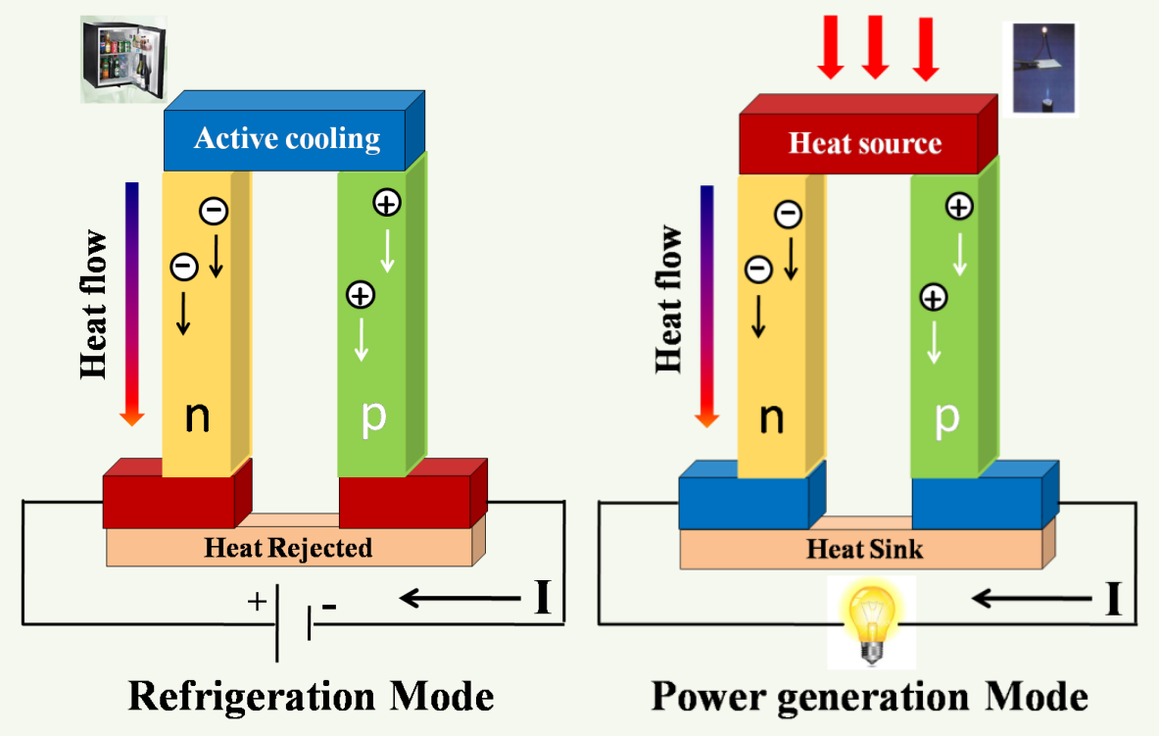
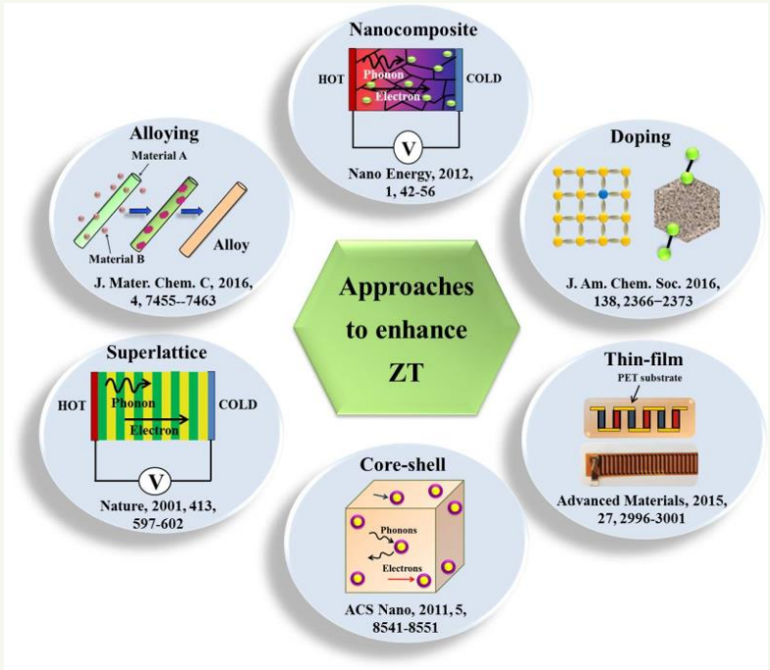
Introduction



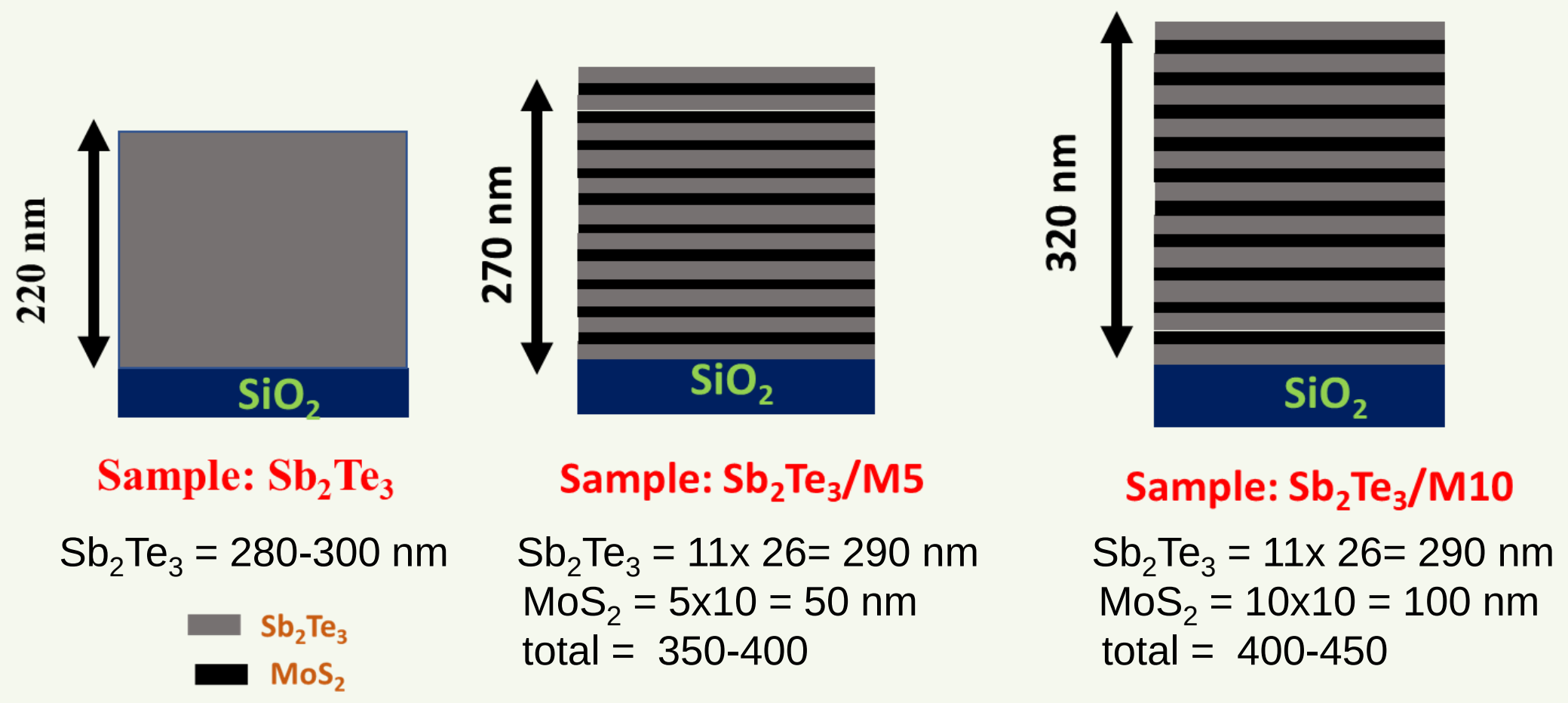
The two operational modes of Thermoelectric device



Various Approaches employed to enhance ZT values.

The concept of thermoelectricity is paramount for both resolving issues related to energy crisis and as well as solutions for global heat management. However, the inadequacy in the value of figure of merit (FOM) still restricts its use in commercial applications and cannot currently compete with the existing techniques.

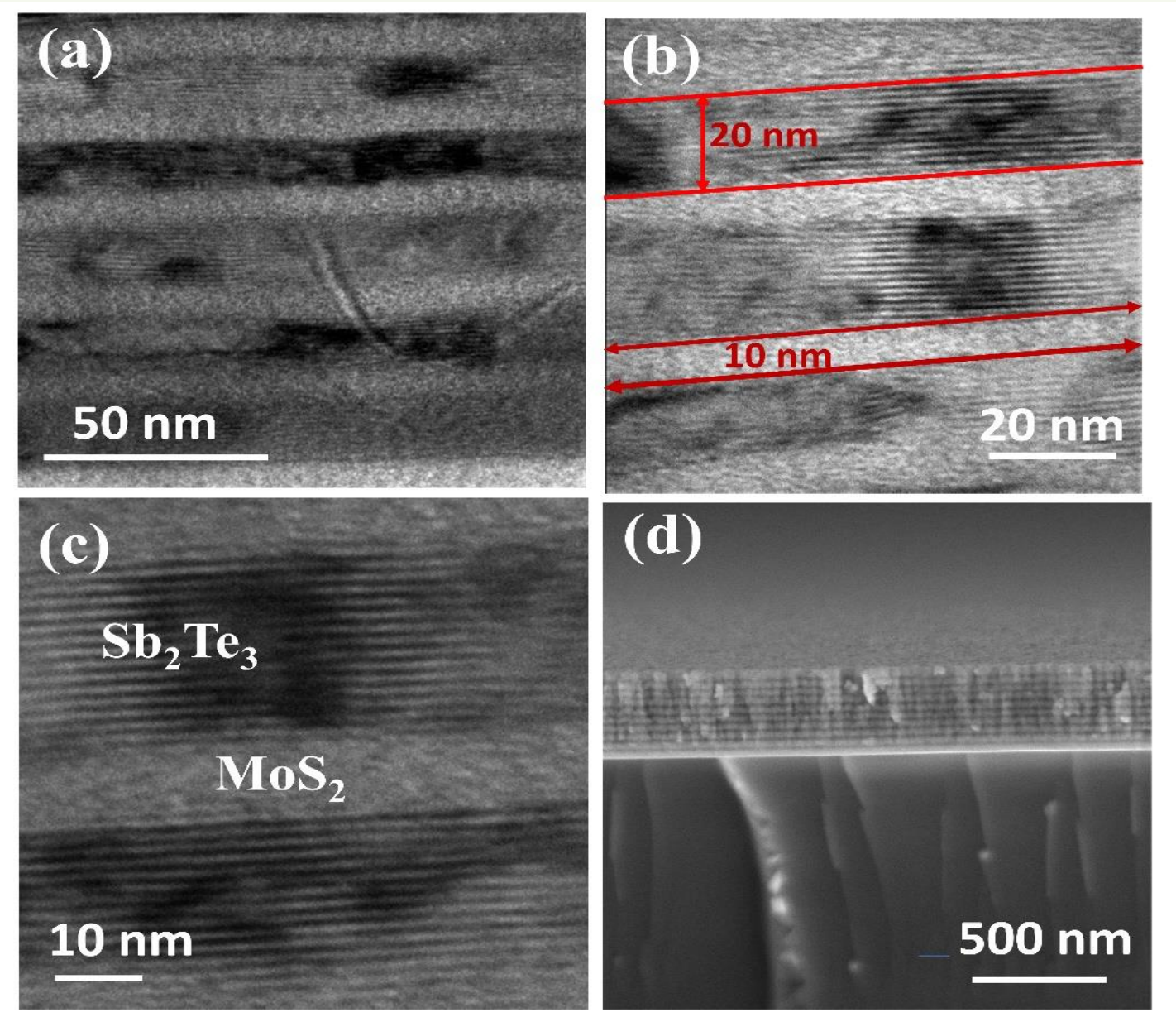
Methodology



Sb_2Te_3 = 280-300 nm

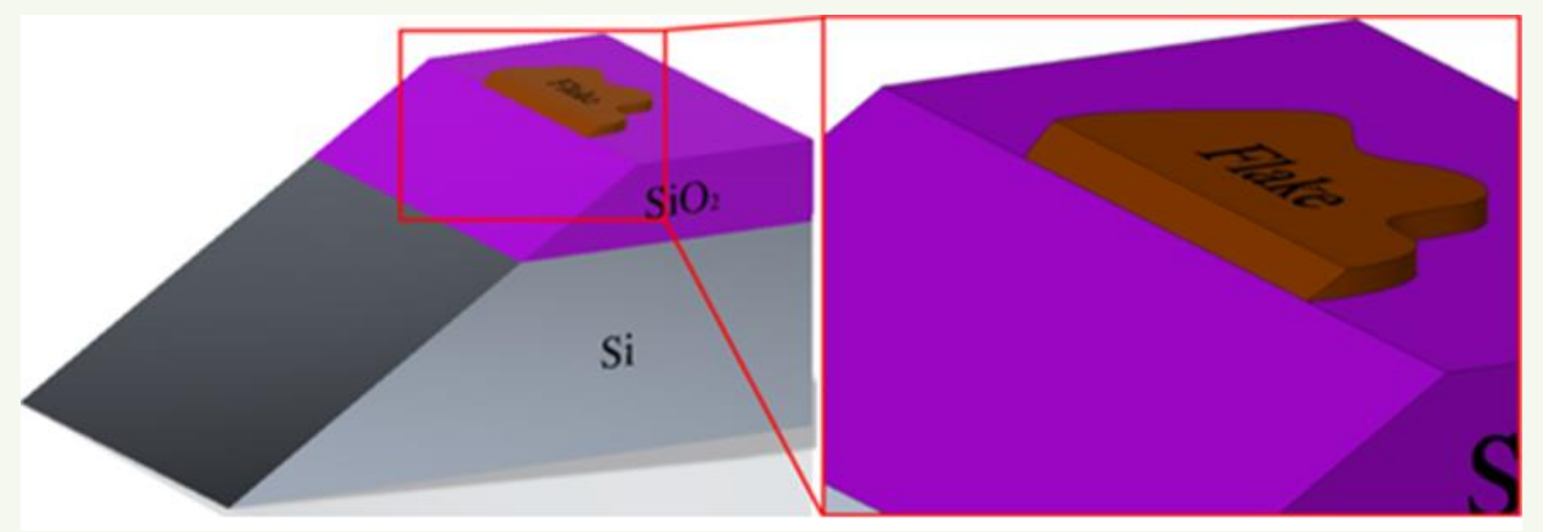
Sb_2Te_3 = 11x 26= 290 nm
MoS_2 = 5x10 = 50 nm
total = 350-400

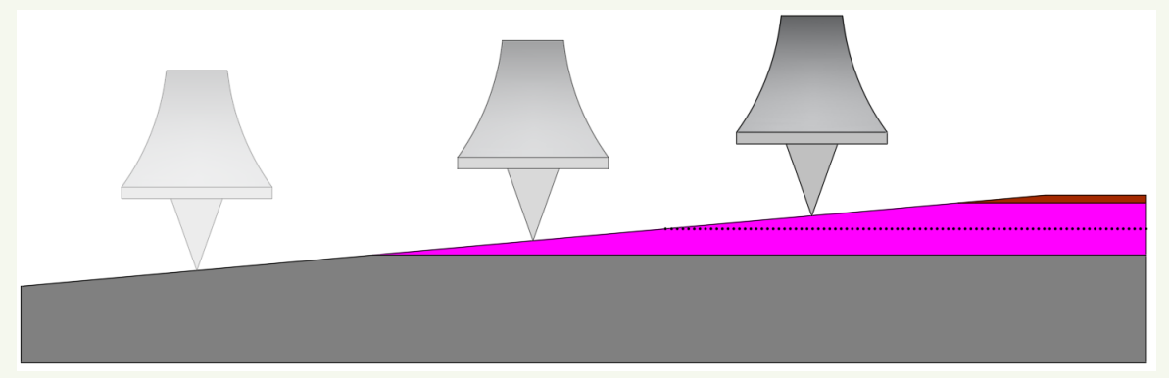
Sb_2Te_3 = 11x 26= 290 nm
MoS_2 = 10x10 = 100 nm
total = 400-450



(a)-(c) HRTEM images of Sb_2Te_3/M10 multilayer sample with different magnification and (d) the cross-section FESEM image.

- Sb_2Te_3/MoS_2 multilayer structures were fabricated with varying thickness of MoS_2 layers.
- The electrical and thermal transport was analysed as a function of number and thickness of MoS_2 layers.
- KPFM results show the presence of a potential barrier for majority carrier holes.
- The samples were prepared by Beam Exit Cross-sectional polishing (BEXP) which uses Ar ions to create a near-atomically flat low angle (1 to 5°) wedge shaped oblique cut with minimal sample damage.
- The measurement of thermal resistance on wedge samples allows to separate the contribution from the interfacial thermal resistance and to independently quantify in-plane and across-the-plane values of thermal conductivity via simple analytical model.



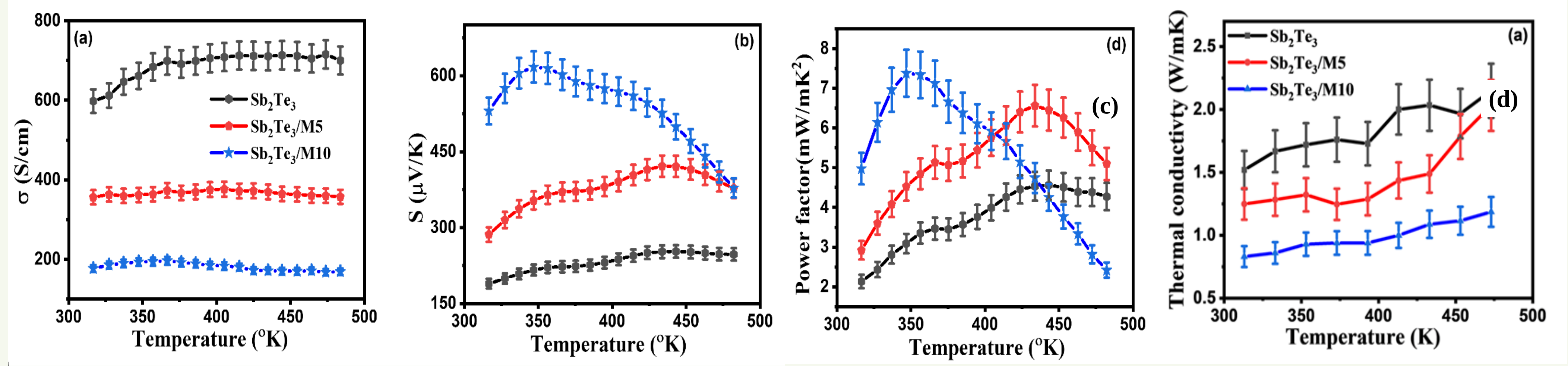


For bulk isotropic material and a contact radius above the phonon mean free path, the thermal spreading resistance is given by $R_S = \frac{1}{4\kappa a}$ .With small angle wedge cut each InSe measurement point can be approximated as a layer of variable thickness. We can then use the transverse isotropic model for R_S for the heat spreading within the layer on a substrate

$$R_{S(t)} = \frac{1}{\pi\kappa_1 a}\int_0^\infty \left[\frac{1+Kexp\left(-\frac{2\xi teff}{a}\right)}{1-Kexp\left(-\frac{2\xi teff}{a}\right)}\right] J1(\xi)\sin(\xi)\frac{d\xi}{\xi^2}$$

Muzychka, Y. S., et al. (2004). J Thermophys Heat Transfer 18(1): 45-51.

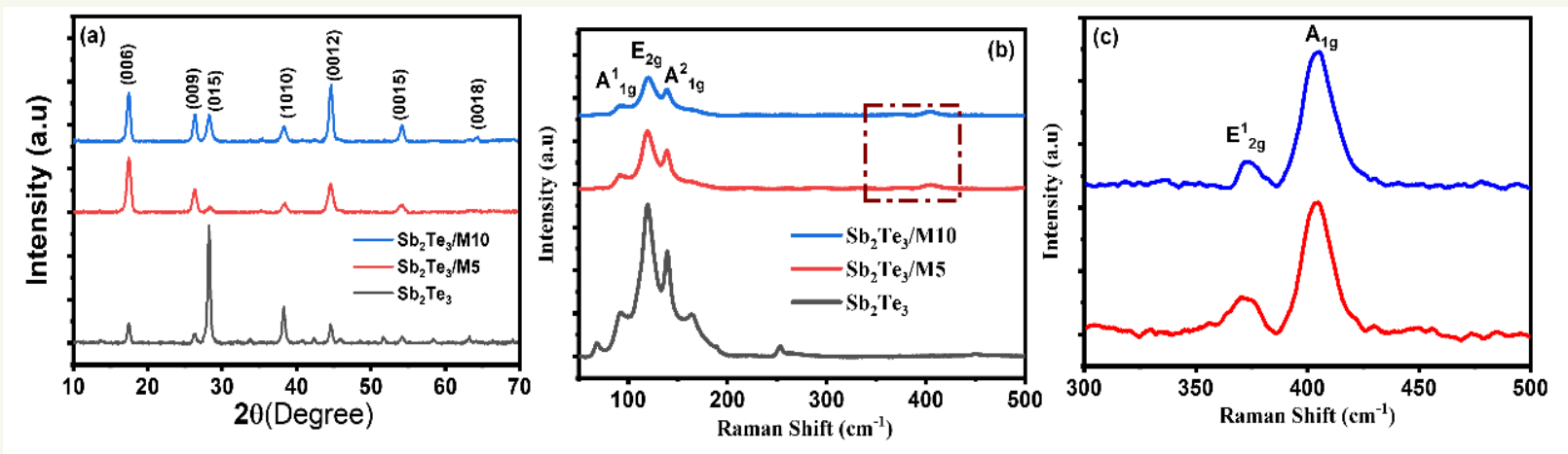
Results



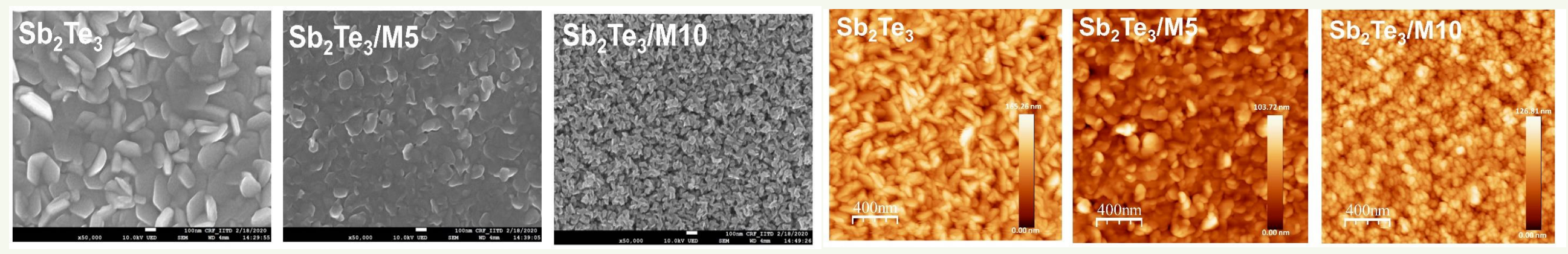
Thermoelectric properties of the Sb_2Te_3 and Sb_2Te_3/MoS_2 multilayer samples with the temperature range 320-484 K (a) electrical conductivity, (b) Seebeck coefficient and (c) power factor and (d) thermal conductivity measured by 3ω method.

The carrier concentration, electrical conductivity, Seebeck coefficient, Hall mobility and power factor values of Sb_2Te_3 and Sb_2Te_3/MoS_2 samples at room temperature.

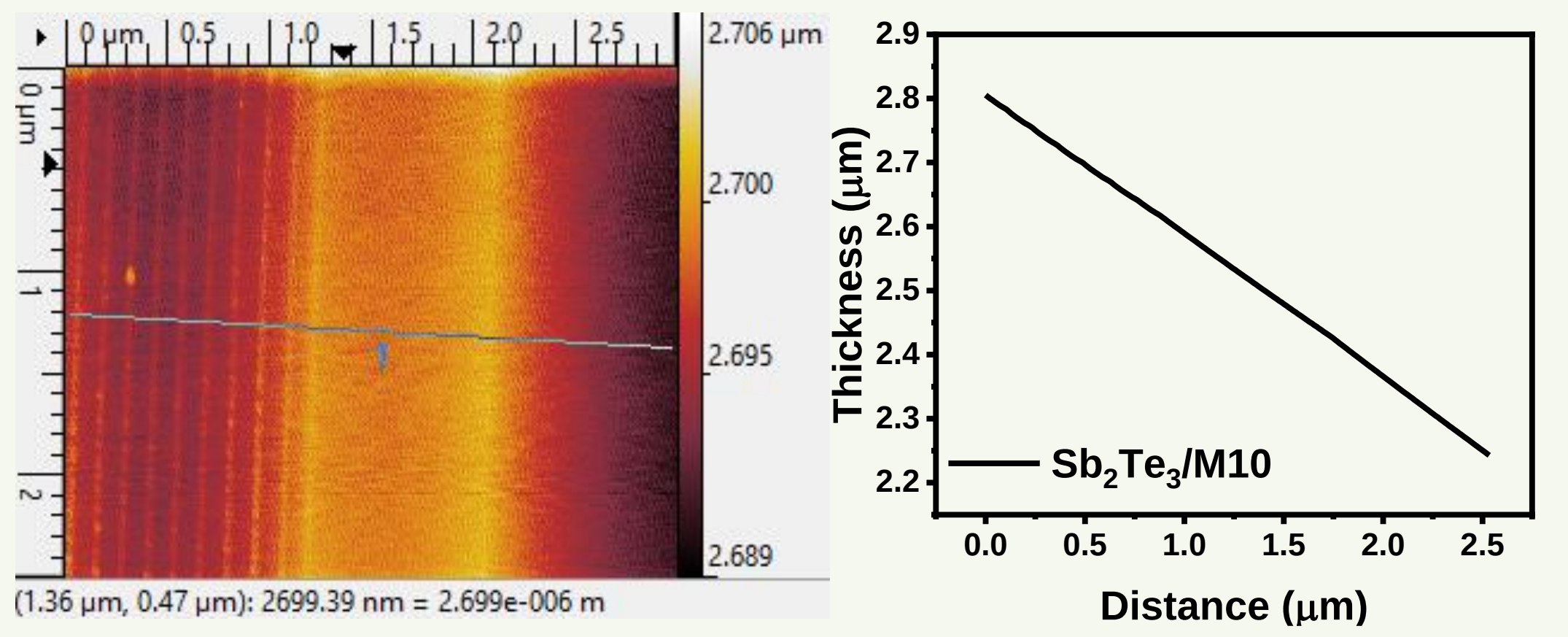
Sample Name	Carrier concentration 10^{19} (cm^{-3})	Electrical conductivity (S/cm)	Hall mobility (cm^{2}V^{-1}S^{-1})	Seebeck coefficient (µV/K)	Power factor (mW/mK^2)
Sb_2Te_3	13.5	688	35.16	188.23	2.09
Sb_2Te_3/M5	4.8	357.93	46.84	286.76	2.9
Sb_2Te_3/M10	1.9	180.86	59.49	531.07	4.99



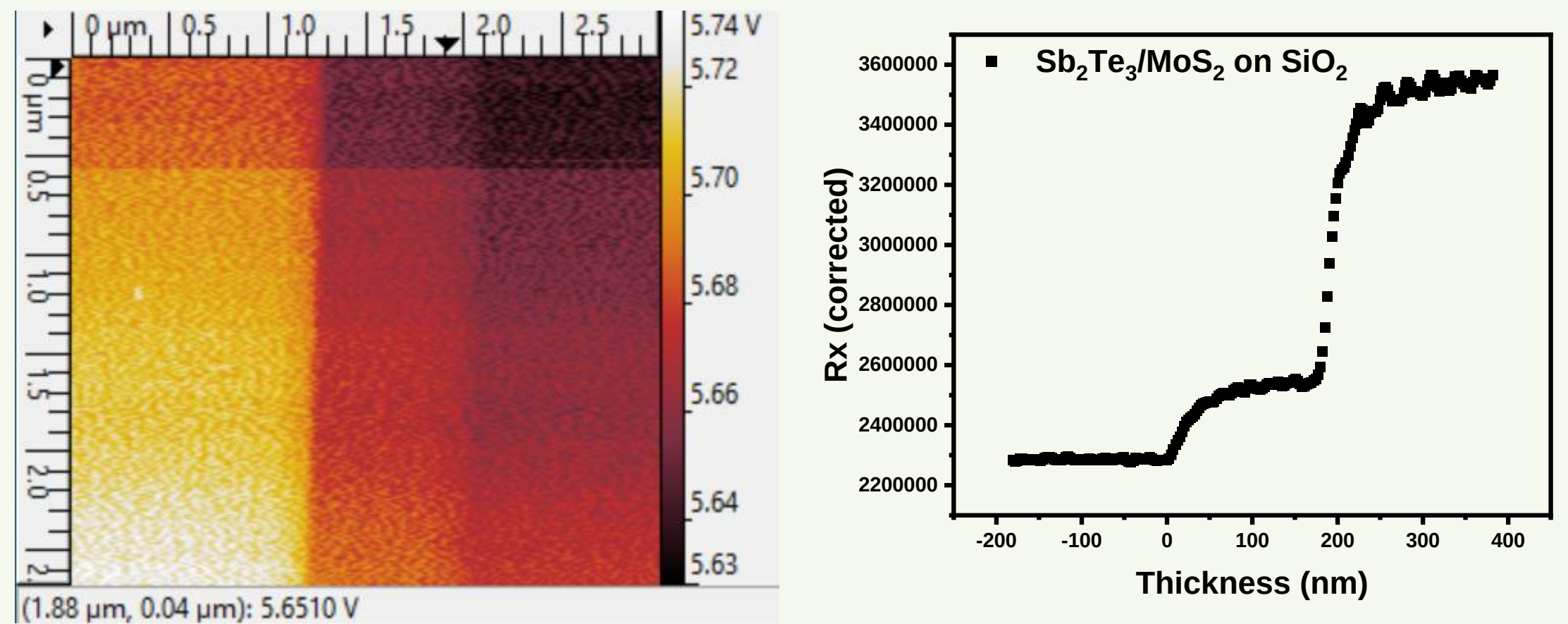
(a) X-ray diffractogram, (b) Raman measurements of Sb_2Te_3, Sb_2Te_3/MoS_2 and (c) the zoom of Raman spectra.



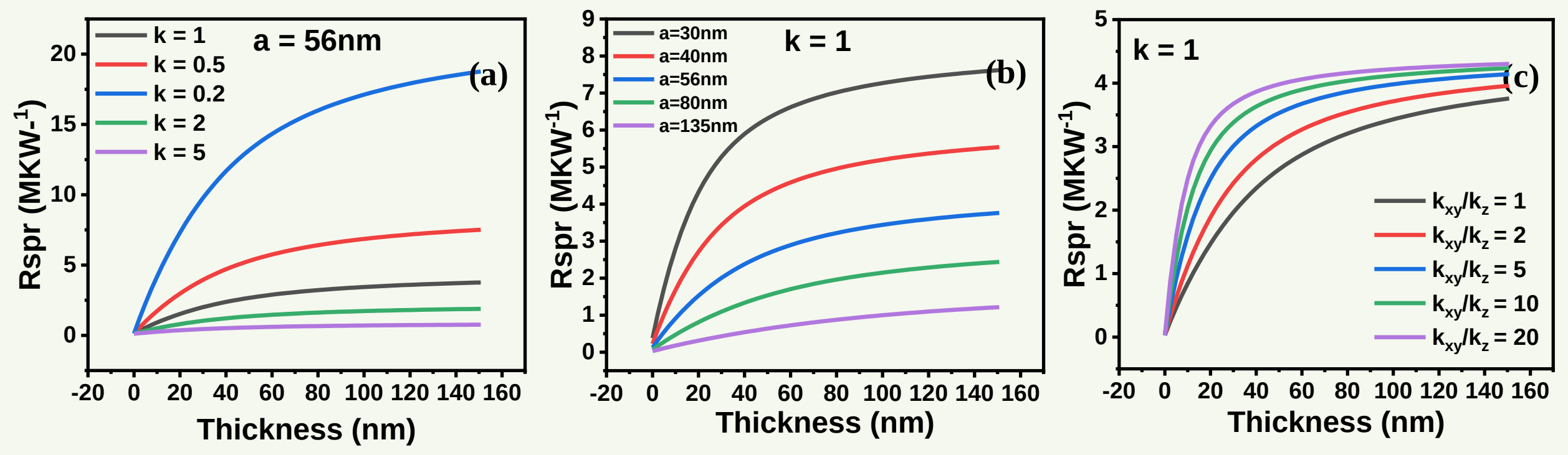
FESEM micrographs and AFM surface topography of Sb_2Te_3 and Sb_2Te_3/MoS_2 multilayer thin film samples



Topography image and profile of wedge cut Sb_2Te_3/M10 sample on SiO_2 substrate having different thickness.



Thermal image and thermal profile of wedge cut Sb_2Te_3/M10 sample on SiO_2 substrate having different thickness.



Simulated curves for Muzychka Method, depicting the dependence of the curve on (a) the value of a, (b) the value of k and (c) anisotropic nature of the material

- The simulated curves were generated by varying a, k1 and ratio of kxy/kz.
- For Anisotropic model, k1 and teff in Muzychka equation is substituted by k1= $\sqrt{kxy * kz}$ and teff = t/($\sqrt{kz/kxy}$).

Conclusions

- High Seebeck coefficient value (619 µV/K at 347 K) was observed along with lower thermal conductivity values (0.83 mW/mK^2 at RT) for Sb_2Te_3/M10 multilayer samples.
- The present work highlights the direct importance of interfaces and the possibility of further improving the thermoelectric response of the material.

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