Supporting Information

$(Bi_xSb_{1-x})_2Se_3$ thin films for short wavelength infrared region solar cells

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Supporting information S1

Table S1. Composition of $(Bi_xSb_{1-x})_2Se_3$ thin film obtained by CSS method.

X_{target} = *Bi/(Bi + Sb)*	**0.00**	**0.10**	**0.30**	**0.50**	**0.65**
X_{exp} = *Bi/(Bi + Sb)*	0.00	0.01 ± 0.003	0.02 ± 0.01	0.06 ± 0.01	0.07 ± 0.01
Se/(Bi + Sb)	1.53 ± 0.06	1.55 ± 0.03	1.60 ± 0.03	1.50 ± 0.02	1.50 ± 0.06
X_{target} = *Bi/(Bi + Sb)*	**0.75**	**0.85**	**0.95**	**1.00**	
X_{exp} = *Bi/(Bi + Sb)*	0.11 ± 0.01	0.20 ± 0.01	0.30 ± 0.01	1	
Se/(Bi + Sb)	1.33 ± 0.06	1.45 ± 0.03	1.46 ± 0.05	1.66 ± 0.09	

Supporting information S2

To quantitatively understand the behaviour of the preferred orientation, the texture coefficient (TC) of the Sb_2Se_3 thin film has been calculated using equation (S1)

$$TC_{hkl} = \frac{I_{hkl}}{I_{0,hkl}} / \frac{1}{N} \sum_{i=1}^{N} \frac{I_{h_ik_il_i}}{I_{0,h_ik_il_i}} \qquad \text{(S1)}$$

Where I_{hkl} is the intensity of the diffraction peaks corresponding to hkl reflection $I_{o,hkl}$ is the intensity of hkl reflection of the standard Sb_2Se_3 (JCPDS no. 051-0861). N is the number of reflections considered for the calculation.

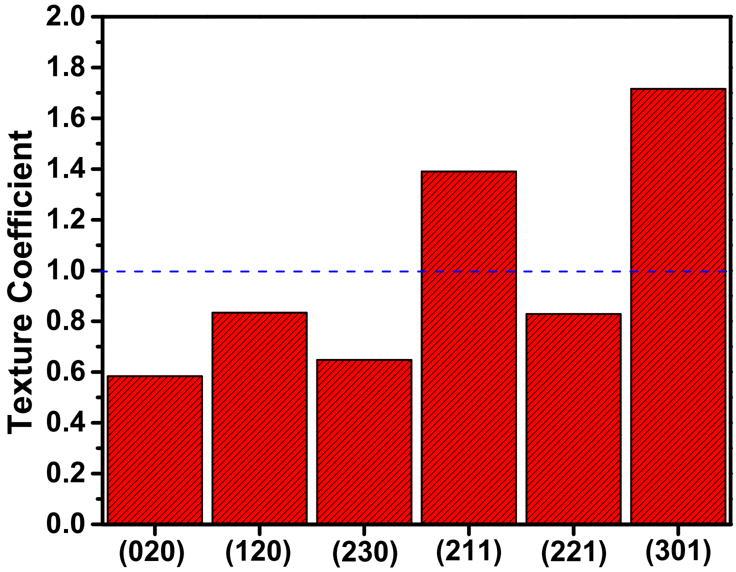

Figure S2. Texture coefficient (TC) of the Sb2Se3 thin-film estimated for (hk0) and (hk1) family of planes

Supporting information S3

Williamson-Hall Method

Crystallite domain size and microstrain in the thin films were estimated from the XRD peak broadening.

$$\beta_l = \frac{k\lambda}{L\ cos\theta} \qquad (1)$$

$$\beta_e = 4\varepsilon\ tan\theta \qquad (2)$$

Here, wavelength of X-ray λ = 1.5406 Å, L = crystallite domain size, K = 0.94, β_l = peak broadening due to crystallite dome size, ε = microstrain, β_e = peak broadening due to micro strain. θ = Bragg diffraction angle

Total boarding in the XRD peaks is the sum of (1) and (2)

$$\beta_{total} = \beta_l + \beta_e = \frac{k\lambda}{L\ cos\theta} + 4\varepsilon\ tan\theta$$

$$\beta_{total}\ cos\theta = \frac{k\lambda}{L} + 4\varepsilon\ sin\theta \qquad (3)$$

If was make a plot between $\beta_{total}\ cos\theta$ and $4sin\theta$ than the intercept on the y-axis will give the crystallite domain size, and the slope will give us microstrain present in the film.

Here, β_{total} is the full width at half maximum after subtracting the instrument broadening β_i. The instrument broadening $\beta_i$was estimated after subtracting the FWHM of the standard silicon reference sample as per the (4). Here $\beta$is the FWHM of the XRD peaks of $(Bi_xSb_{1-x})_2Se_3$ thin film

$$\beta_{total} = \sqrt{(\beta - \beta_i)\sqrt{\beta^2 - \beta_i^2}} \qquad (4)$$

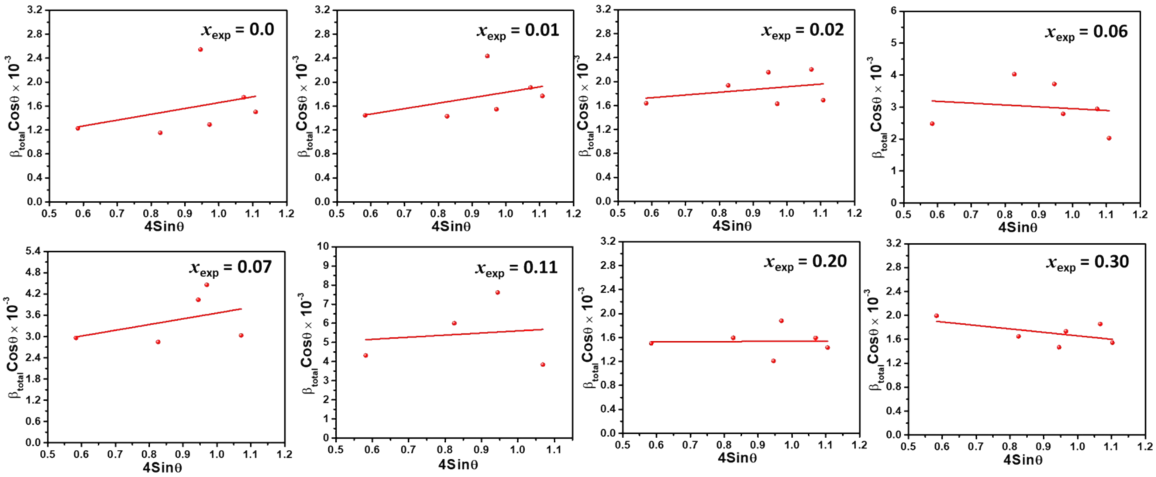

Figure S3. The plots of β_{total}Cosθ versus 4Sinθ for $(Bi_xSb_{1-x})_2Se_3$ thin films. Strain is extracted from the slop, and crystallite site is extracted from the y-intercept.

Supporting information S4

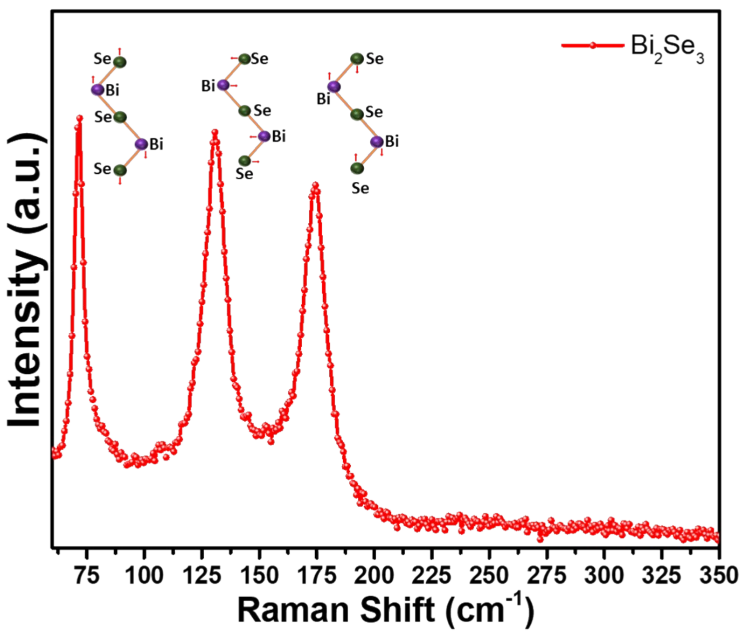

Figure S4. Raman spectrum of the Bi_2Se_3 thin film. Inset is the vibrational modes of Bi_2Se_3 [1-2].

1. H.H. Kung, M. Salehi, I. Boulares, A.F. Kemper, N. Koirala, M. Brahlek, P. Lošťák, C. Uher, R. Merlin, X. Wang, S.W. Cheong, S. Oh, G. Blumberg, Surface vibrational modes of the topological insulator Bi_2Se_3 observed by Raman spectroscopy, Phys. Rev. B. 95 (2017). https://doi.org/10.1103/PhysRevB.95.245406.
2. J. Zhang, Z. Peng, A. Soni, Y. Zhao, Y. Xiong, B. Peng, J. Wang, M.S. Dresselhaus, Q. Xiong, Raman spectroscopy of few-quintuple layer topological insulator Bi_2Se_3 nanoplatelets, Nano Lett. 11 (2011) 2407–2414. https://doi.org/10.1021/nl200773n.

Supporting information S5

The optical bandgap of the $(Bi_xSb_{1-x})_2Se_3$ thin films was estimated by measuring the diffuse reflectance on UV-Vis-NIR spectrophotometer.

Using Kubelka-Munk (KM) function the reflectance spectrum can be transformed to the corresponding absorbtion spectrum using eq. (1) [1]

(1) $$F(R) = \alpha/S = (1 - R)^2/2R]$$

Using Tauc method the energy dependent absorbction coefficient (α) can be expressed by following eq. (2) [2-3]

(2) $$(\alpha h\nu)^{\frac{1}{n}} = B(h\nu - E_g)$$

Combining eq1 and eq2

(3) $$[F(R)h\nu]^{\frac{1}{n}} = B(h\nu - E_g)$$

The value of n is equal to 1/2 or 2 for the direct and indirect transition bandgaps, respectively.

The bandgaps were estimated by a linear fit of the linear part of the KM plot. Errors for the bandgaps are estimate by shifting the fitting range by ± 10 meV.

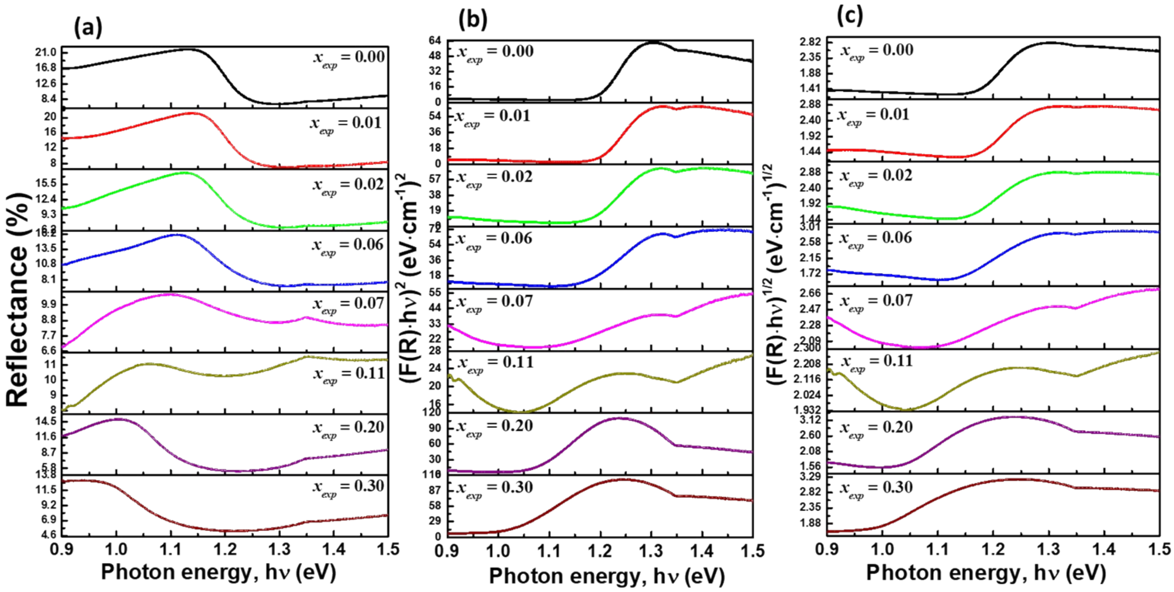

Figure S5. (a) Measured diffused reflectance and (b) and (c) shows the corresponding KM function for the estimation of direct and indirect bandgap, respectively.

1. E.N. Davis, Developments in Applied Spectroscopy, Springer US, 1965. https://doi.org/10.1007/978-1-4684-8691-9
2. J. Tauc, R. Grigorovici, A. Vancu, Optical Properties and Electronic Structure of Amorphous Germanium, Phys. Status Solidi. 15 (1966) 627–637. https://doi.org/10.1002/pssb.19660150224.
3. N.F. Mott, E.A. Davis, Conduction in non-crystalline systems V. Conductivity, optical absorption and photoconductivity in amorphous semiconductors, Philos. Mag. 22 (1970) 903–922. https://doi.org/10.1080/14786437008221061.

Supporting information S6

Table S6. $(Bi_xSb_{1-x})_2Se_3$ thin film solar cell performance parameters. *PCE* is power conversion efficiency, J_{sc} is short circuit current, *FF* is fill factor, R_{sh} is shunt resistance, R_s is series resistance.

x_{exp}	J_{sc} (mA/cm^2)	V_{oc} (mV)	*FF* (%)	*PCE* (%)	R_{sh} (Ω·cm^2)	R_s (Ω·cm^2)
0.00	0.68 ± 0.28	187.42 ± 46.21	31.04 ± 2.64	0.68 ± 0.28	25.75 ± 8.59	10.68 ± 2.52
Best cell	**14.19**	**244.95**	**35.23**	**1.23**	**31.33**	**8.40**
0.01	3.14 ± 0.64	39.33 ± 5.23	23.74 ± 0.22	0.03 ± 0.009	12.46 ± 1.39	13.31 ± 1.42
Best cell	**3.67**	**45.4**	**23.57**	**0.039**	**11.99**	**12.78**
0.02	21.72 ± 1.93	139.96 ± 5.9	28.79 ± 0.69	0.88 ± 0.10	8.32 ± 0.65	4.81 ± 0.59
Best cell	**22.73**	**146.04**	**29.15**	**0.97**	**8.41**	**4.56**
0.06	16.16 ± 1.03	136.45 ± 0.0354	27.90 ± 1.43	0.633 ± 0.216	10.19 ± 2.88	6.33 ± 1.09
Best cell	**17.14**	**169.52**	**29.63**	**0.861**	**13.11**	**6.53**
0.07	18.68 ± 8.71	59.87 ± 0.01	25.23 ± 0.33	0.27 ± 0.11	4.39 ± 2.59	4.02 ± 2.29
Best cell	**27.78**	**54.34**	**24.94**	**0.376**	**2.00**	**1.88**