

Electronic supplementary information (ESI)

**Stability & Durability of Self-Driven Photo-detective Parameters
based on $\text{Sn}_{1-\beta}\text{Sb}_\beta\text{Se}$ ($\beta = 0, 0.05, 0.10, 0.15, 0.20$) Ternary Alloys
Single Crystals**

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Table. S1. The growth parameters fixed for crystal growth of $\text{Sn}_{1-\beta}\text{Sb}_{\beta}\text{Se}$ ($\beta = 0, 0.05, 0.10, 0.15, 0.20$)

Sample $\text{Sn}_{\beta}\text{Sb}_{1-\beta}\text{Se}$	Compound		Crystal Growth Process		
	Temperature (K)	Time (h)	Temperature		Heating rate (k/h)
			Source Zone	Growth Zone	
$\beta = 0$	1073	160	1073	1023	20
$\beta = 0.05$	1093	160	1093	1043	20
$\beta = 0.10$	1093	160	1093	1043	20
$\beta = 0.15$	1093	160	1093	1043	20
$\beta = 0.20$	1093	160	1093	1043	20

Table. 1 presents the growth parameters of the $\text{Sn}_{\beta}\text{Sb}_{1-\beta}\text{Se}$ ($\beta = 0, 0.05, 0.10, 0.15$ and 0.20) crystals. Which confirms the high temperature and prolonged time durations of the growth of materials.

Table.S2. Atomic percentage data obtain from EDAX spectra of as grown $\text{Sn}_{1-\beta}\text{Sb}_\beta\text{Se}$ ($\beta = 0, 0.05, 0.10, 0.15, 0.20$) crystals.

Sample $\text{Sn}_{1-\beta}\text{Sb}_\beta\text{Se}$	Element	Wt. (%) of constituents taken for growth	Wt. (%) of constituents obtained from EDAX
$\beta = 0$	Sn	60.05	57.50
	Se	39.94	42.50
$\beta = 0.05$	Sn	58.01	54.59
	Se	38.91	42.18
	Sb	03.07	03.23
$\beta = 0.10$	Sn	53.96	51.18
	Se	38.88	41.28
	Sb	07.15	07.54
$\beta = 0.15$	Sn	52.67	50.31
	Se	37.12	38.06
	Sb	10.21	11.63
$\beta = 0.20$	Sn	50.89	49.06
	Se	35.83	36.75
	Sb	13.28	14.19

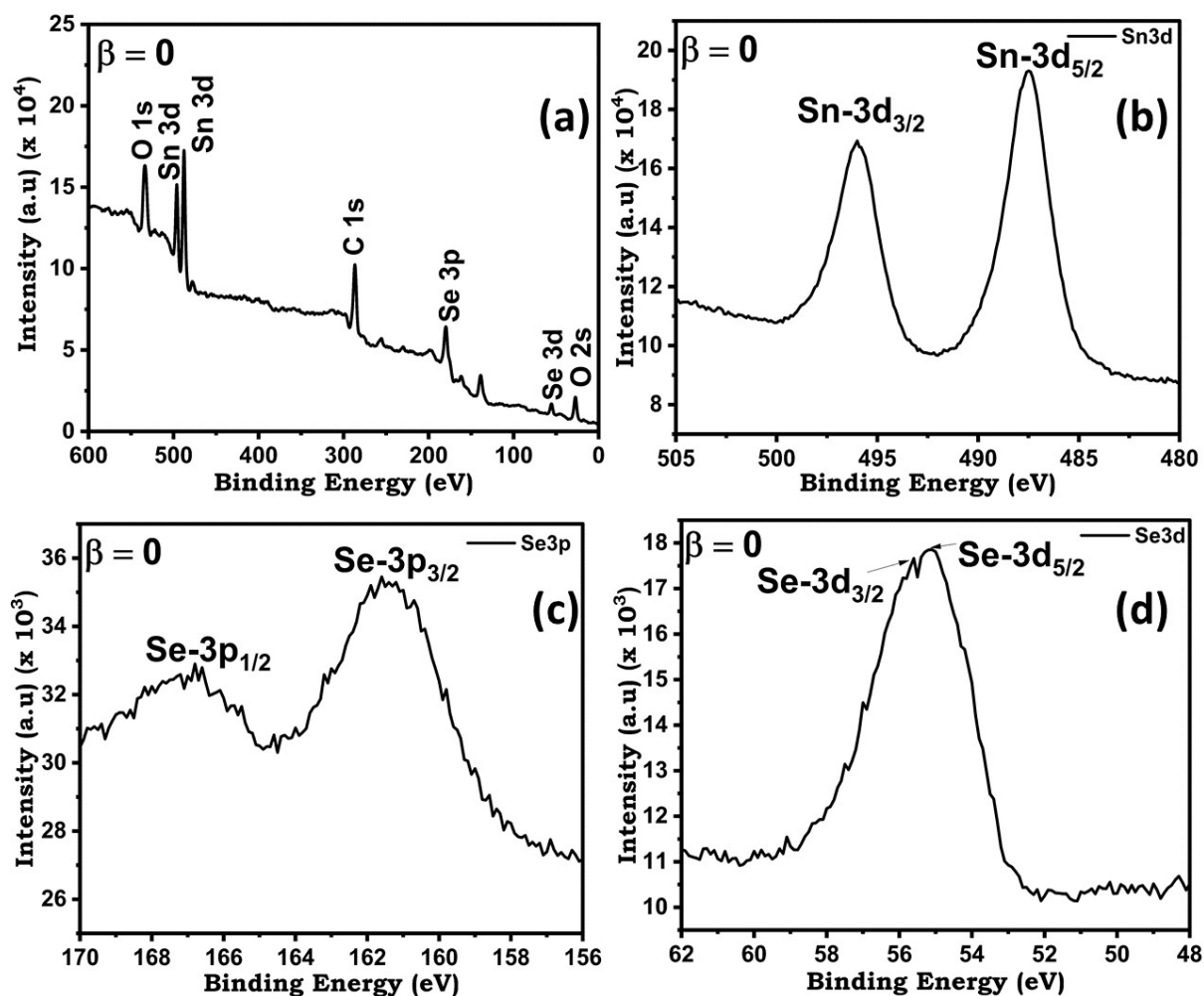
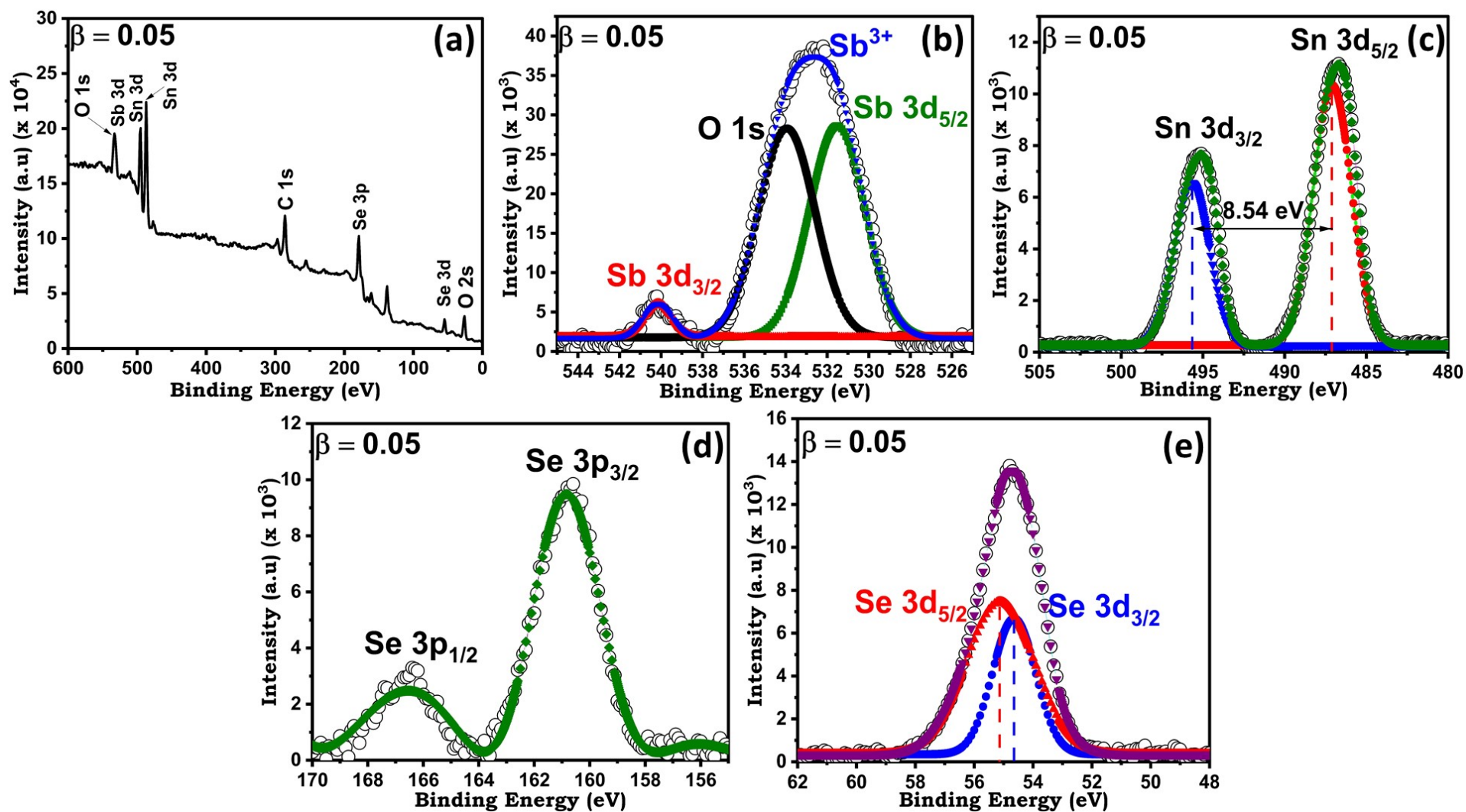
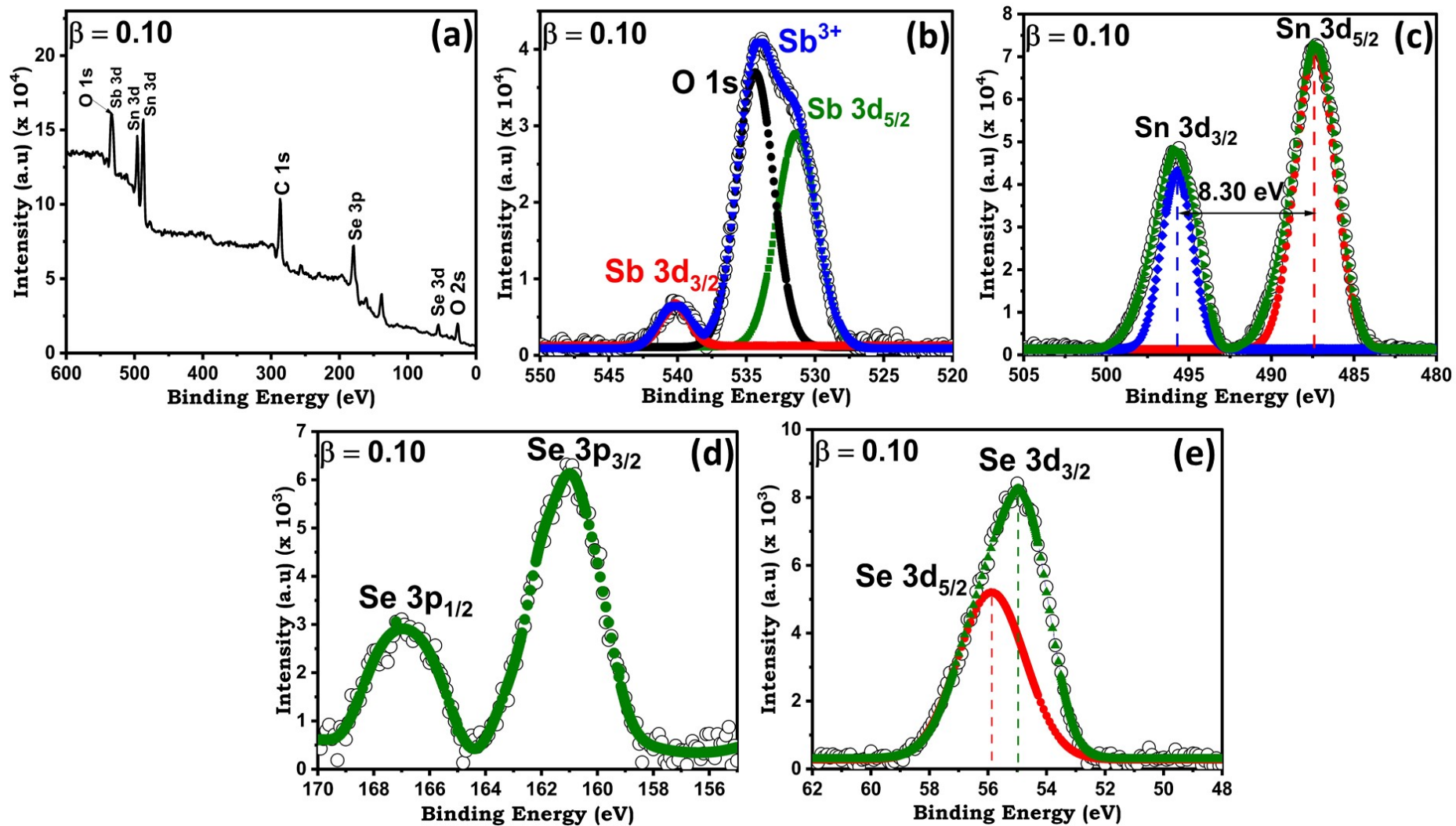
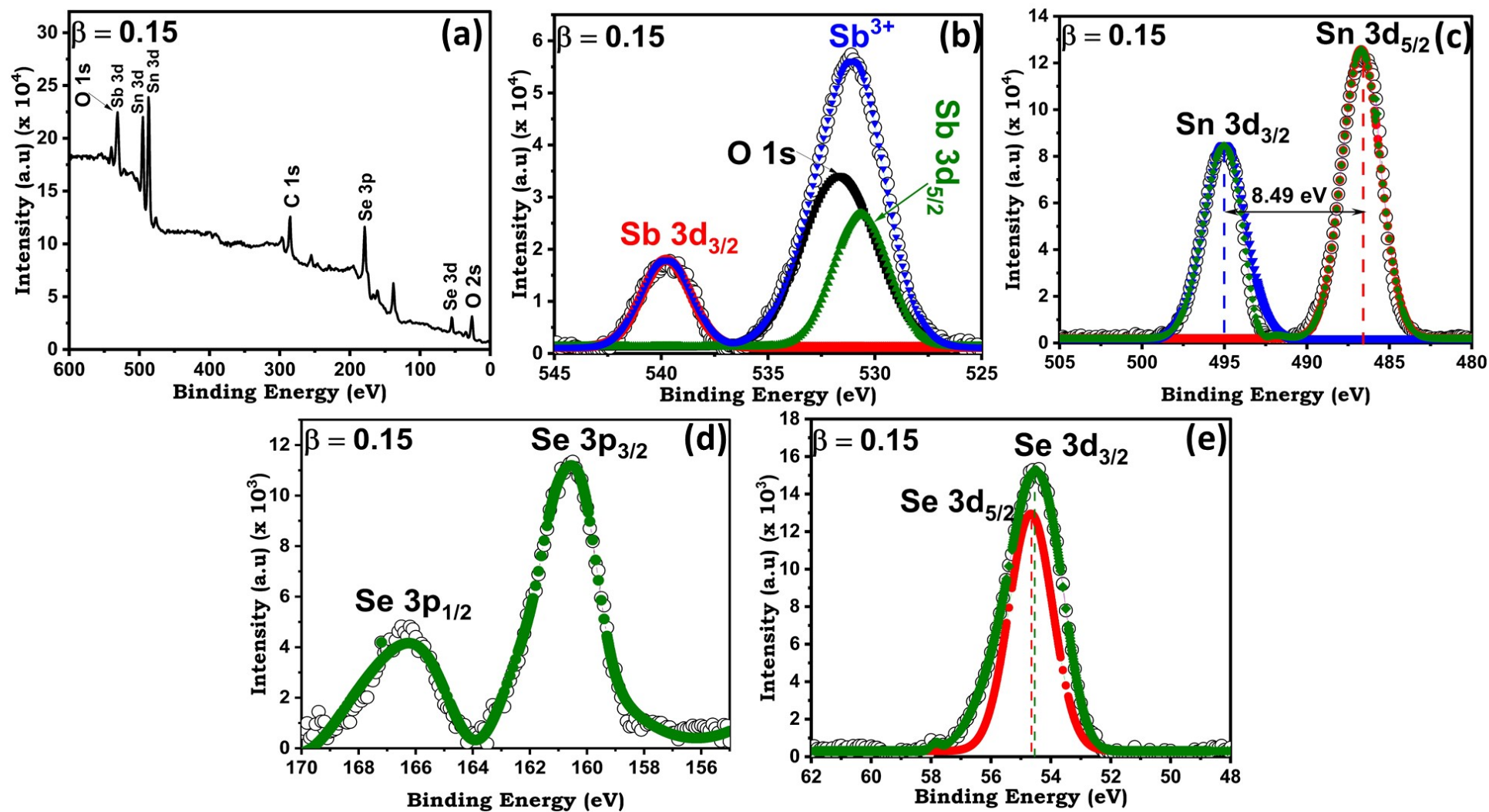


Figure. S1. (a) The XPS full range spectra of SnSe crystal for (b) Se 3d_{3/2} & 3d_{5/2} (c) Se 3p_{3/2} & 3p_{1/2} and (d) Sn 3d_{5/2} & 3d_{3/2}.

Figure 1a indicates the full range spectra of the SnSe ternary alloys. Where binding energy peaks of Se and Sn are observed to be matching with the reported articles. Figure 1b indicates the peaks at ~496 eV and ~487 eV correspond to Sn 3d_{3/2} and Sn 3d_{5/2} doublets, which is associated with the Sn+4 oxidation state. The peak at ~160.84 eV and ~166.45 eV corresponds to Se 3p_{3/2} and 3p_{1/2} doublet state depicted in Fig. 3c. While Figure 1d indicates the singlet peaks of Se 3d_{3/2} and Se 3d_{5/2} at ~56.... eV and ~55.... eV corresponding to 3d_{5/2} and 3d_{3/2}, respectively, which is attributed to the Sn+4 oxidation state.¹

Figure. S2. The XPS Spectra of Sb_{0.05}Sn_{0.95}Se crystal.

Figure. S3. The XPS Spectra of Sb_{0.10}Sn_{0.90}Se crystal.

Figure. S4. The XPS Spectra of Sb_{0.15}Sn_{0.85}Se crystal.

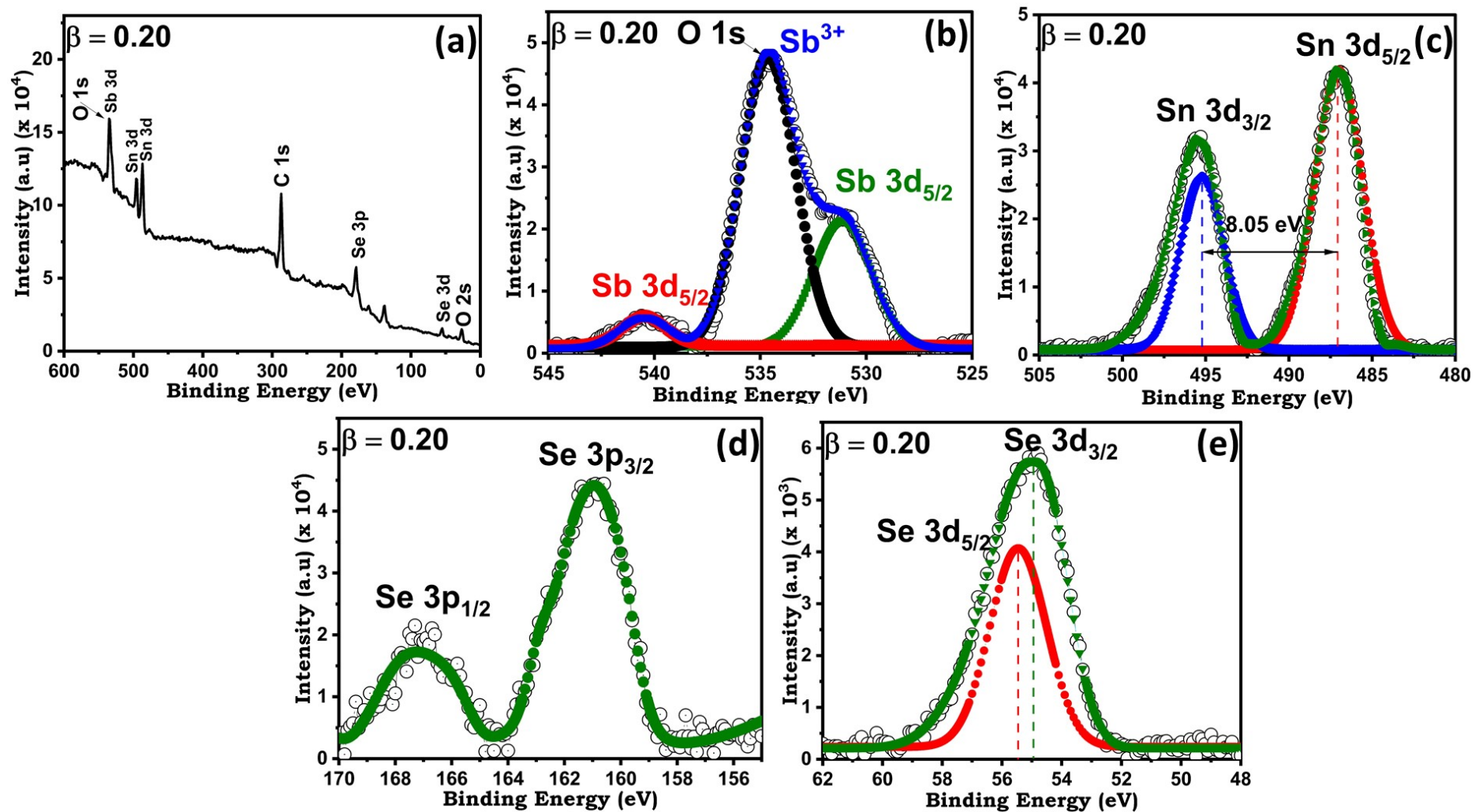
Figure. S5. The XPS Spectra of Sb_{0.20}Sn_{0.8}Se crystal.

Figure 2 to 5 show the XPS spectra obtained to analyze chemical states and to confirm the formation of the prepared Sn Sb Se ternary alloys.

Figure 2 to 5 (b) indicates the peaks of Sb at ~540 eV, ~535 eV and ~530 eV correspond to Sb 3d3/2, Sb+3 and Sb 3d5/2 (tabulated in manuscript table 1), which is associated with the Sb+3 oxidation state. Other peak of O 1s presents oxygen states.

XRD equations:

The structural parameters including crystallite size (τ) for the most preferred orientation were assessed using the 'Debye-Scherrer' formula given in below:

$$D = \frac{0.9 \lambda}{\beta_{2\theta} \cos \theta} \quad (1)$$

Where ' λ ' is the wavelength of the X-Ray source, ' $\beta_{2\theta}$ ' is the broadening of the diffraction line measured at half of its maximum intensity (FWHM) and ' θ ' is the Bragg's angle in degrees.

The crystallite size was calculated by resolving the most intense peak from the XRD graphs. The micro-strain evaluated in the crystals was evaluated from the equation:

$$\varepsilon = \frac{\beta_{2\theta} \cos \theta}{4} \quad (2)$$

Where ' $\beta_{2\theta}$ ' is the broadening of the diffraction line measured at half of its maximum intensity (FWHM) and ' θ ' is Bragg's angle in degrees.

The dislocation density (δ) defined as the length of dislocation lines per unit volume of the crystals is calculated for all planes using the equation:

$$\delta = \frac{15 * \varepsilon}{a * D} \quad (3)$$

Where ' ε ' is the micro-strain, obtain from further equations, a is the lattice parameters and 'D' is the crystallinity size obtained from the 'Debye-Scherrer' formula.^{2,3}

Table.S3. The XRD parameters of $\text{Sn}_{1-\beta}\text{Sb}_\beta\text{Se}$ ($\beta = 0, 0.05, 0.10, 0.15, 0.20$) crystals.

Sample $\text{Sn}_{1-\beta}\text{Sb}_\beta\text{Se}$	Lattice Parameter			c/a	Volume (\AA^3)	FWHM	2θ (Degree)	d	Crystallite size t (nm)	Micro Strain ϵ ($\text{lin-}2\text{m-}4$)	Dislocation Density $\delta \times 10^{14}$ ($\text{lin m-}4$)
	A	B	C								
$\beta = 0$	11.490	4.440	4.135	0.35988	210.95	0.4000	31.074	0.287572	35.964	0.09635	3.507
$\beta = 0.05$	11.485	4.435	4.130	0.35960	210.366	0.4100	31.095	0.287446	35.088	0.09875	3.684
$\beta = 0.10$	11.480	4.430	4.125	0.35932	209.783	0.4200	31.108	0.287389	34.254	0.10115	3.868
$\beta = 0.15$	11.475	4.425	4.125	0.35948	209.455	0.4300	31.112	0.287236	33.458	0.10356	4.055
$\beta = 0.20$	11.460	4.410	4.110	0.35864	207.714	0.4500	31.138	0.287001	14.387	0.10837	9.862

Figure. S6. The optical microscopic images of $\text{Sn}_{1-\beta}\text{Sb}_\beta\text{Se}$ ($\beta = 0, 0.05, 0.10, 0.15, 0.20$) crystals.

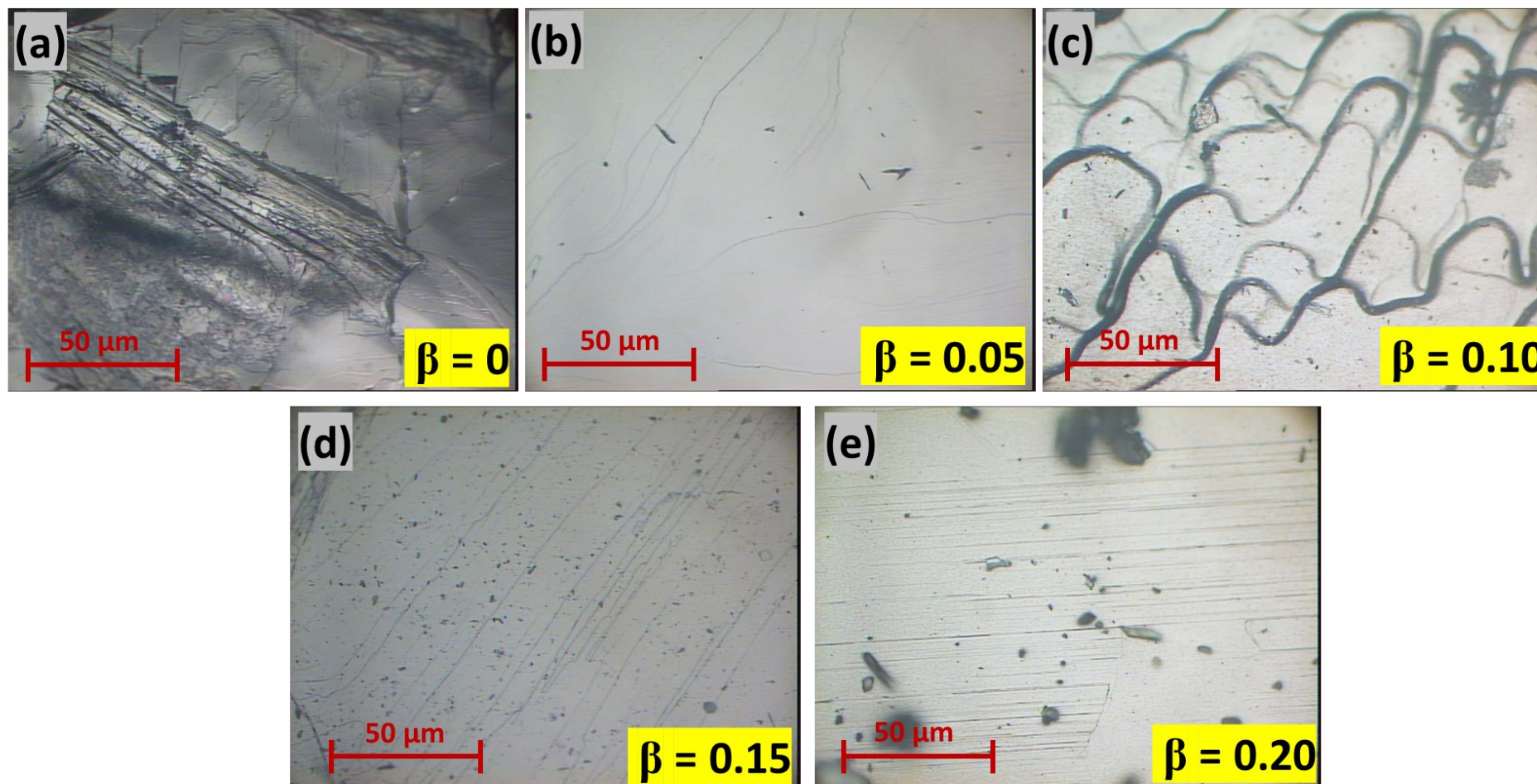


Figure 5 shows the optical microscopic images of the Sn Sb Se ternary alloys. Here fig. 1a shows the layered surfaces, 1b shows the flat region of as-grown crystals, 1c shows the layered surfaces, 1d shows the many layered grown crystals and 1e shows the layered surface of the as-grown crystals. There are cleaved surfaces to show the layered and flat region to fabricate the devices of these samples.

UV VIS equations:

The optical absorption (α) was calculated using Lambert law as shown in the equation:

$$\ln\left(\frac{I_0}{I}\right) = 2.303 A = \alpha t \quad (4)$$

$$\alpha = \frac{2.303 * A}{t} \quad (5)$$

Where, α is the absorption, I_0 and I are the intensity of incident and transmitted light, respectively t is the thickness of the crystals and A is the optical absorbance.

The band gap of SnSe thin film can be determined by the below equation:

$$(\alpha h\nu)^n = A (h\nu - E_g) \quad (6)$$

Where E_g is the band gap, A is the constant that comes from the Fermi-Golden rules, and n depends on the type of the band transition of the materials.

The indirect band gap was calculated using the Davis-mott model (for $n = \frac{1}{2}$). The indirect energy gap is given generally by the below equation:

$$E_g' = \frac{E_1 + E_4}{2} = \frac{E_2 + E_3}{2} \quad (9)$$

The phonon energies are given below equations:

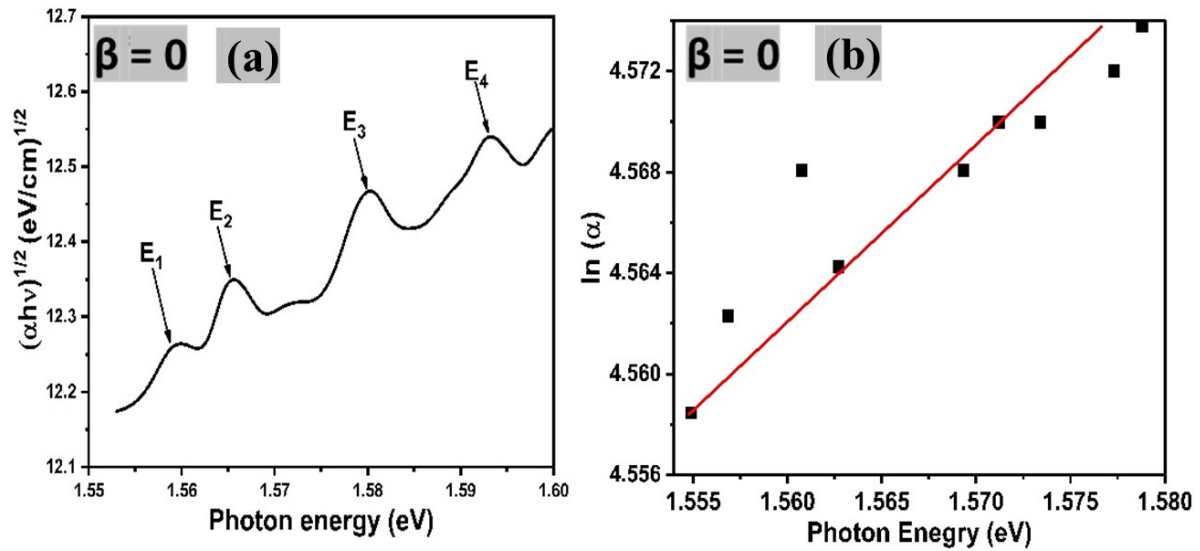
$$E_{p1} = \frac{E_4 - E_1}{2} \quad \text{and} \quad E_{p2} = \frac{E_3 - E_2}{2} \quad (10)$$

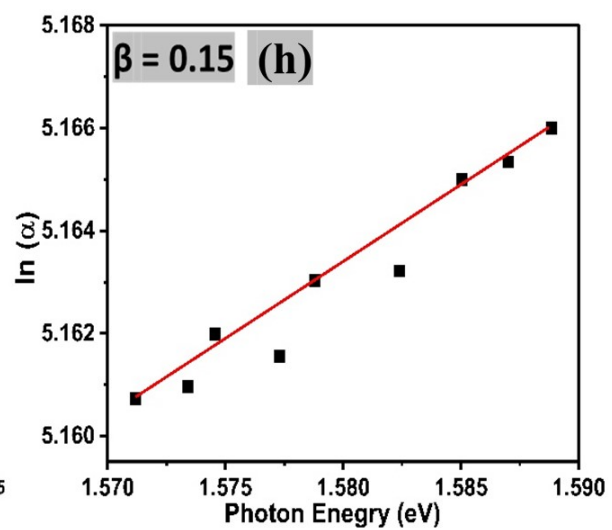
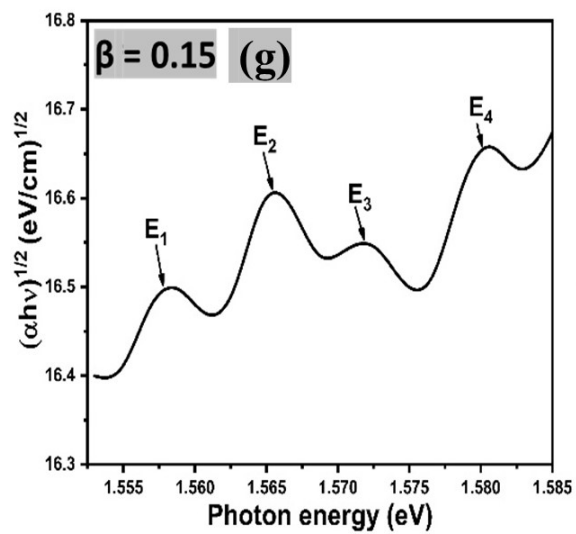
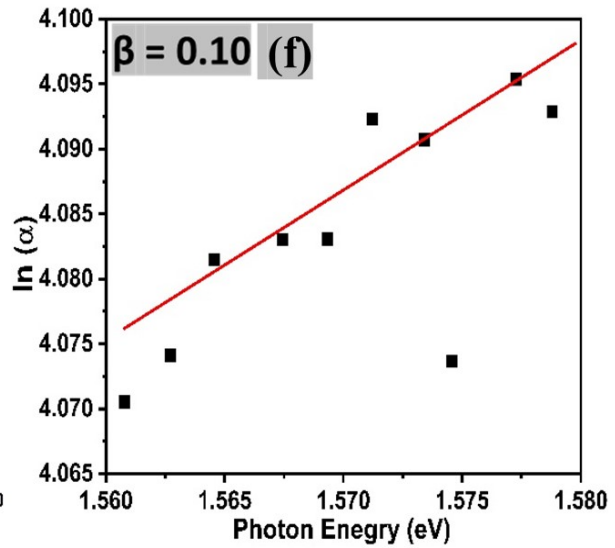
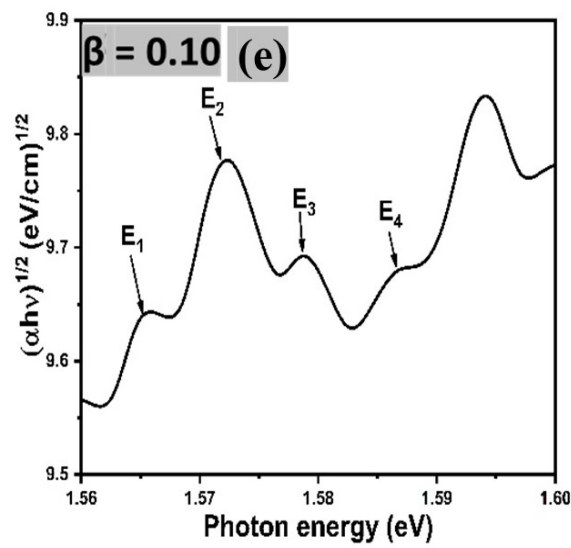
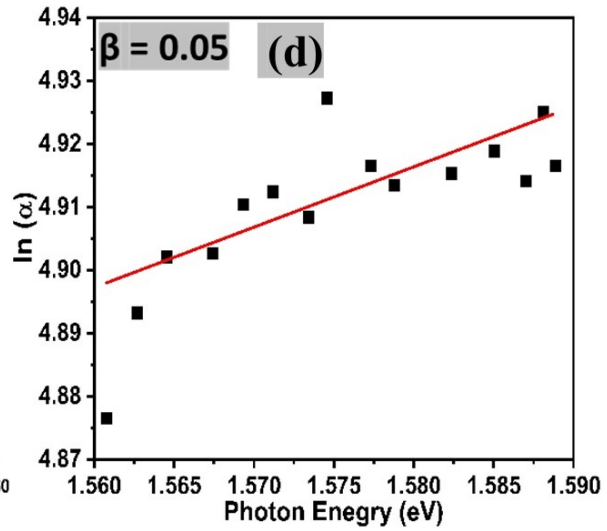
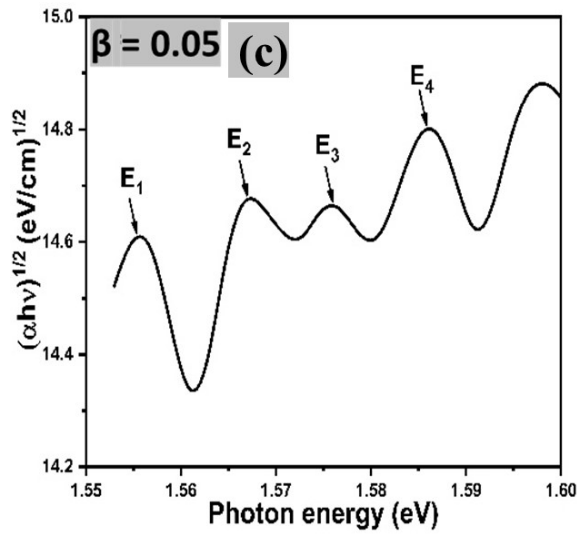
where $E'g$ is the energy band gap due to absorption and emission of phonon energies, and E_{p1} and E_{p2} are the absorbed and emitted phonon energies.

The steepness constant is determined usually using the equation shown below

$$\sigma = \frac{K_B T}{E_U} \quad (11)$$

where ' K_B ' is the Boltzmann constant, ' E_U ' the Urbach energy, and ' T ' the temperature in Kelvin (K).³⁻⁷





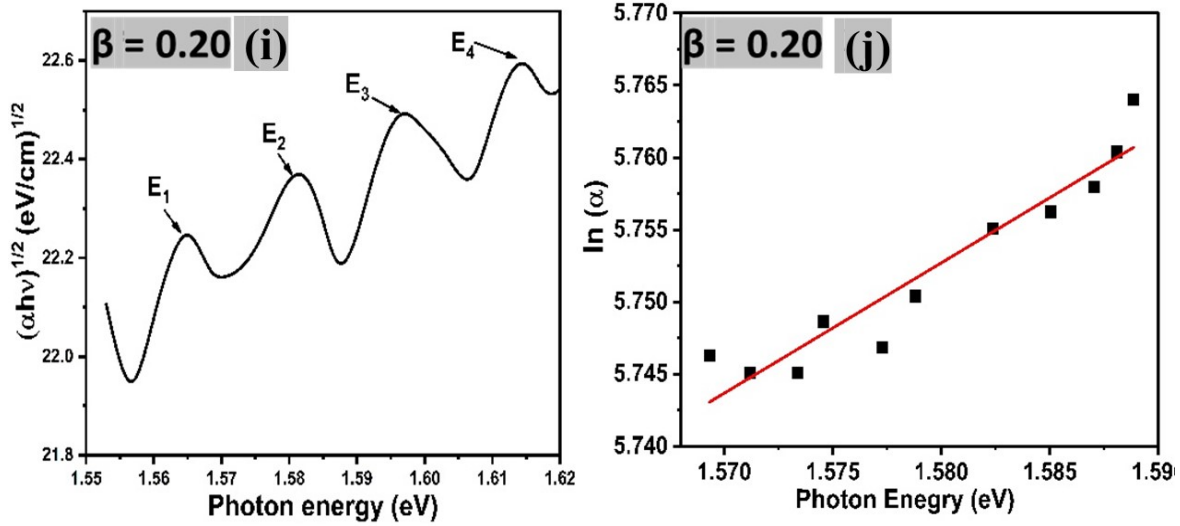


Figure. S7. (a-j) The energy stack and urbach energy of $\text{Sn}_{1-\beta}\text{Sb}_\beta\text{Se}$ ($\beta = 0, 0.05, 0.10, 0.15, 0.20$) crystals.

Pulse photodetectors equations:

The detector parameters such as photocurrent (I_{ph}), sensitivity (S), responsivity (R_λ), and specific detectivity (D) are evaluated using the following equations:

$$I_{ph} = I_{ill} - I_{dark} \quad (12)$$

$$S = \frac{I_{ph}}{I_{dark}} \quad (13)$$

$$R_\lambda = \frac{I_{ph}}{P \cdot A} \quad (14)$$

$$D = \frac{R_\lambda S^{1/2}}{(2eI_{dark})^{1/2}} \quad (15)$$

Where I_{ill} = current under illuminated condition and I_{dark} = current under dark condition) is the photocurrent, P is the illumination intensity, A is the effective area of the photodetector, λ is the wavelength of the light source, h is Planck's constant, e is the elementary electronic

charge (1.6×10^{19} C), c is the speed of light in vacuum, k is the wavelength of incident radiation, and I_{dark} is the dark current.^{8–10}

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