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The microstructural parameters analysis of SnSe_{0.2}S_{0.8} thin film

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Abstract. Sn(S_{0.8}Se_{0.2}) thin films were successfully grown by evaporation technique with the distance variation between substrate and source (10, 15, and 25 cm) to investigate their microstructural parameters and morphology. The X-ray diffraction patterns showed that Sn(S_{0.8}Se_{0.2}) thin film had a single phase with the orthorhombic crystal structure. The crystallite size and the lattice strain were evaluated using the Williamson-Hall (W-H) analysis with Uniform Deformation Model (UDM). The increase of the spacer ($d = 10, 15, \text{ and } 25 \text{ cm}$) causes the increase of the value of strain and crystallite size. One of the factors that affect the increase of crystallite size in the SnSe_{0.2}S_{0.8} thin films with the spacer is the lattice strain value of the crystals. The scanning electron microscopy (SEM) confirmed the high homogeneity of grains. SnSe_{0.2}S_{0.8} thin films contain Stannum (Sn) at 21.88 %, Selenium (Se) at 2.31 %, and Sulfur (S) elements at 14.24 % in the majority.

1. Introduction

Nowadays, the compound of layered semiconductors of tin sulfide (SnS) and tin selenide (SnSe) has garnered immense attention due to their wide applications, particularly in solar cells application [1]. SnS with orthorhombic structure has a high absorption coefficient, which accounts for 10^4 cm^{-1} and it is suitable as a light-absorbing material for solar cell application [2,3]. SnS is one of the promising compounds due to low cost with the band gap energy about 1.5 eV which is the optimum band gap for solar cell application [2,4]. Likewise, SnSe is a binary IV-VI semiconductor of *p*-type having band gap about 1.35 eV with a high optical absorption coefficient of 10^5 cm^{-1} . In addition, SnSe is abundant in nature and non-toxic [5–7].

The properties of SnS and SnSe thin films, i.e., crystal structure, optical band gap, and electrical characteristics depend on the preparation methods. The various deposition techniques of thin film growth have been carried out, such as chemical bath deposition [8], electrodeposition [9], vacuum evaporation [10], and chemical vapour depositions (CVD) [11]. Among the various methods, vacuum evaporation was employed to grow SnSeS thin films due to producing good quality of thin films with the simple process and economical costs [12]. Improvements of SnSeS thin films structures quality have been conducted such as adjusting substrate temperature during the thin film growth and performing thickness of thin films [1,10]. In addition, Lie, et al carried out the XRD analysis using Rietveld method to obtain detailed structure knowledge [13].



To the best of our knowledge, there are limited previous experimental studies about the effect of spacer between the heat source and substrate during the evaporation process and analysing the microstrain parameters and the crystallite size with W–H approaches. This is one of the important adjustments in the evaporation technique to enhance the quality of SnSeS thin films. If the spacer is too long or too short, SnSeS may not be deposited very well on the preparatory glass substrate. Hence, this paper deals with the spacer effect between the heat source and substrate on the growth of SnSeS thin film. The microstructural parameters of SnSeS thin films i.e the microstrain and the crystallite size were analyzed by Williamson-Hall (W-H) approach and the morphology is discussed in detail.

2. Methods

SnSe_{0.2}S_{0.8} thin films were grown with homemade evaporation technique on preparatory glass with the shallow pressure of diffusion pump. Stannum, selenium, and sulfur were used as primary materials with the mole ratio of 1: 0.2: 0.8, respectively, and heated at a high temperature of about 450 °C on the boat-shaped crucible made of molybdenum (Mo). The preparatory glass was put as a substrate for SnSe_{0.2}S_{0.8} thin films growth with the size of (1.5 × 2) cm². Afterward, a spacer between source and substrate was set with a variation of 10, 15, and 25 cm.

The next step is turning a rotary pump that is capable of suppressing a pressure reaching 10⁻³ torr, and then connected to the secondary pump in the form of a diffusion pump that can decrease the pressure of the evaporator chamber, which accounts for 10⁻⁶ torr. The source of the power supply system was then connected to the crucible to generate electrical currents. The crucible that was filled with materials was set above the spacer purveyed with the electrodes. In case, the electrode was connected to the power supply to adjust the temperature of the substrate.

Finally, the SnSe_{0.2}S_{0.8} put in the crucible was deposited on the preparatory glass substrate. In addition, SnSe_{0.2}S_{0.8} thin films were grown with the preparation parameters as shown in Table 1. The microstructural parameters of SnSe_{0.2}S_{0.8} thin films were then analyzed by XRD Miniflex 600 Rigaku and the morphology of SnSe_{0.2}S_{0.8} thin films were investigated by SEM-EDX JEOL JSM-6510LA.

Table 1. Preparation parameters of SnSe_{0.2}S_{0.8} thin films growth

Parameter	Description
Spacer	10 cm, 15 cm, and 25 cm
Mass of materials	Se: 0.307 g; Sn: 2.308 g; S: 0.498 g
Temperature of substrate	450 °C
Deposition time	8 minutes
Vacuum pressure	4 × 10 ⁻⁵ Torr
Output current	60 A

3. Results and Discussion

To study the effect of a spacer on the microstructural parameters and morphology of SnSe_{0.2}S_{0.8}, different spacer (*d*) between source and substrate in SnSe_{0.2}S_{0.8} thin film growth are studied (spacer = 10 cm, 15 cm, and 25 cm). The XRD patterns of all samples are depicted in Fig 1. All of samples showed the characteristic diffraction peaks corresponding to (120), (101), (111), (140), (200), (141), (211), and (211) planes with the orthorhombic structure [14]. This is in line with the standard JCPDS file no. 39-0354. There are no peaks showing any other element. This is indicated that all of the samples (*d* = 10 cm, 15 cm, and 25 cm) are crystalline.

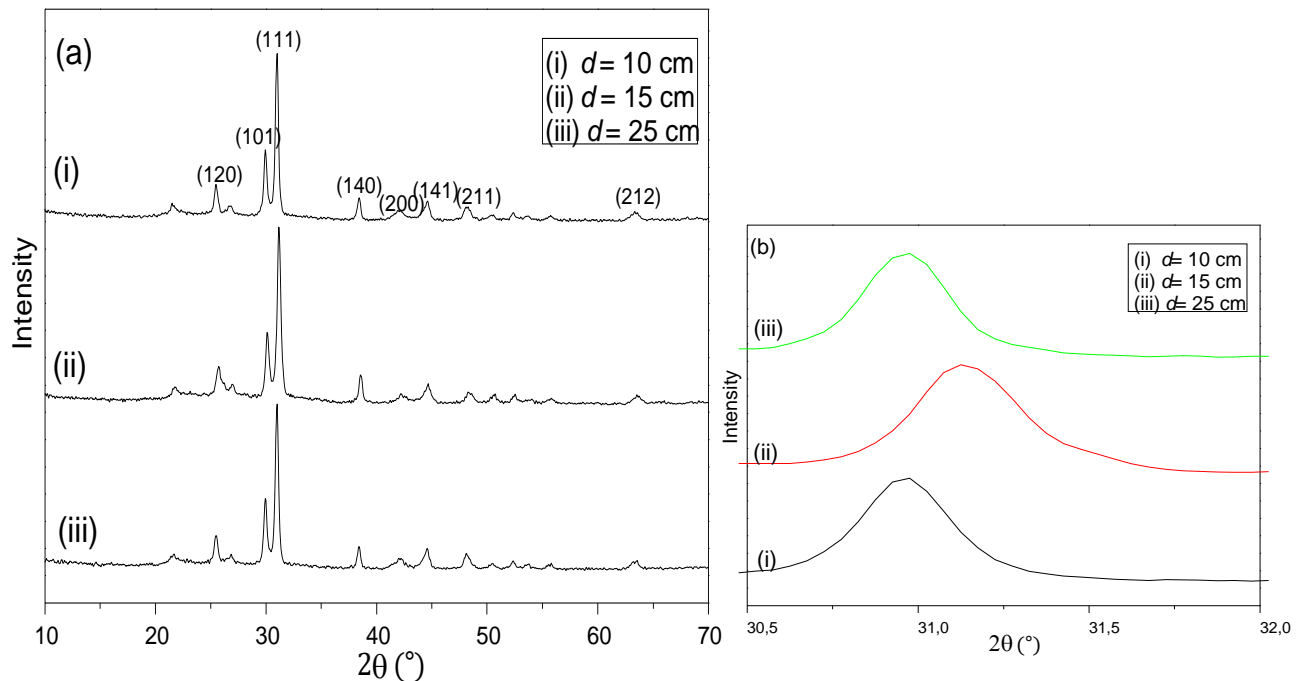


Figure 1. (a) The XRD patterns of SnSe_{0.2}S_{0.8} thin films ($d=10$ cm, 15 cm, and 25 cm), and (b) The enlargement of (111) diffraction peak

Figure 1 (b) displays that the diffraction peak formed in the plane (311) experienced a shift towards a larger diffraction angle along with the increase of spacer while at a spacer of 25 cm the diffraction peak shifted to the smaller diffraction angle. The shift of the diffraction peaks showed the change in the position of the atoms on a lattice. The shift of the diffraction peaks caused the changes in lattice parameter values, strains, and crystallite size.

The strain and crystallite size of SnSe_{0.2}S_{0.8} thin films can be calculated by The Williamson-Hall (W-H) equation. The W-H analysis can be shown with the following equation [15]

$$\beta_{hkl} \cos \theta = \frac{k\lambda}{D} + 4\epsilon \sin \theta$$

The W-H plot of SnSe_{0.2}S_{0.8} thin films for three different spacers is shown in Figure 2. The estimation of crystallite size (D) was obtained from the y -intercept, and the strain (ϵ) from the slope of the linear fit. The above W-H equation represents the UDM (Uniform Deformation Model) which considers the isotropic nature of the crystal. The UDM assumes that strains are in uniform for all crystallographic directions. The UDM analysis in detail is depicted in Table 2.

Table 2. The microstructural parameters of SnSe_{0.2}S_{0.8} thin films at different spacer

Spacer (cm)	Diffraction angle at miller indices 111 (°)	FWHM at miller indices 111 (°)	Crystallite size (nm)	Strain
10	30.97	0.241	42.58	0.0012
15	31.12	0.268	56.658	0.0020
25	30.97	0.238	106.28	0.0034

Table 2 shows the crystallite sizes of the SnSe_{0.2}S_{0.8} thin films at the interval (42.58 – 106.28) nm. The smallest crystallite size is on a sample with a spacer of 10 cm and the highest one is on the sample with a spacer of 25 cm. Overall, it can be seen that by increasing the spacer, the crystallite size of the SnSe_{0.2}S_{0.8} thin films. One of the factors that affect the increase of crystallite size in the SnSe_{0.2}S_{0.8} thin films is the lattice strain value of the crystals and this is in line with the previous result that have investigated [9]. Strains can be stated as a sign of imperfection in a crystal. The greater the strain value, the greater imperfections in the crystal. This is in good agreement with the data as shown in Table 2.

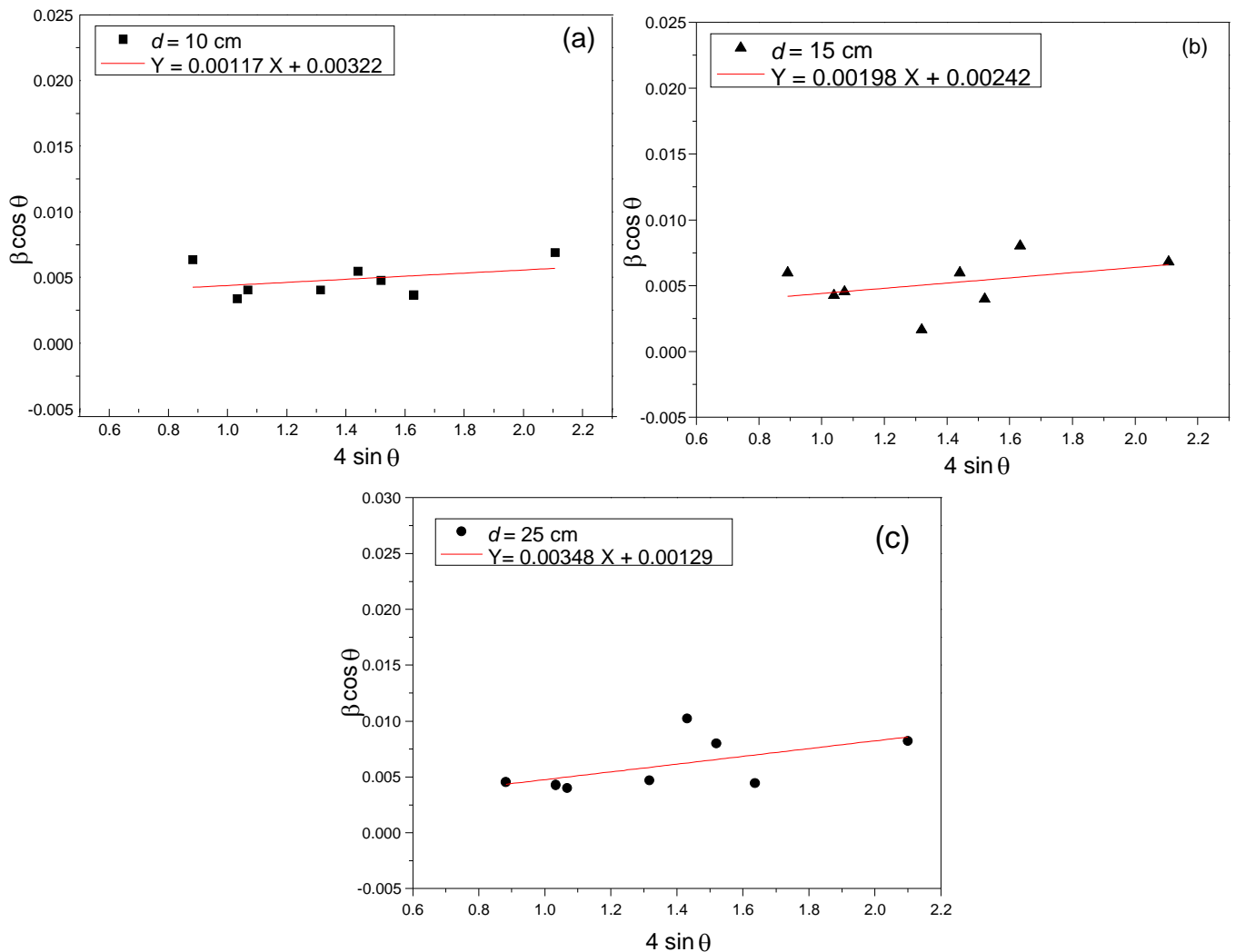
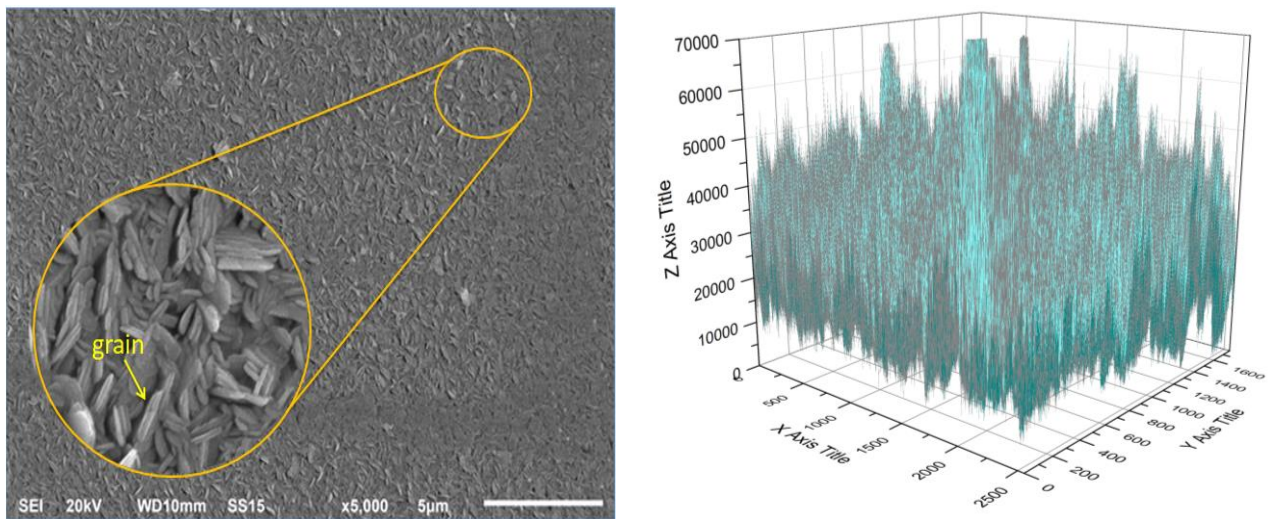


Figure 2. (a) The plot of $\beta_{hkl} \cos(\theta)$ versus $4 \sin(\theta)$ for $\text{SnSe}_{0.2}\text{S}_{0.8}$ thin films at different spacer (a) 10 cm, (b) 15 cm, and (c) 25 cm

The morphology of $\text{SnSe}_{0.2}\text{S}_{0.8}$ thin film for spacer 15 cm is shown in Figure 3.a. It can be seen that the homogeneity of the $\text{SnSe}_{0.2}\text{S}_{0.8}$ crystals formed. The grains are distributed uniformly on the surface. The grain size of the $\text{SnSe}_{0.2}\text{S}_{0.8}$ thin film for spacer 15 cm is about $0.2 \mu\text{m}$. The porosity of the $\text{SnSe}_{0.2}\text{S}_{0.8}$ thin film surface can be calculated by the following formula

$$\phi = 1 - \frac{V_{solid}}{V_{total}}$$

Based on Figure 3.b, the porosity of the surface is obtained 0.683 or 68.33 % with the value of $x_{max} = 2549$ and $y_{max} = 1769$. This result indicates that the surface of $\text{SnSe}_{0.2}\text{S}_{0.8}$ thin film is not totally flat but it has moderate roughness.



(a)

(b)

Figure 3. (a) SEM images and (b) Surface with its coordinates in 3-D for SnSe_{0.2}S_{0.8} thin films at spacer of 15 cm

Figure 4 shows the EDX spectrum of SnSe_{0.2}S_{0.8} thin films at a spacer of 15 cm. Based on the results of EDX characterization, it can be seen SnSe_{0.2}S_{0.8} thin films contain Stannum (Sn) at 21.88 %, Selenium (Se) at 2.31 %, and Sulfur (S) elements at 14.24 % in the majority, while there are other elements such as C, Si, Mo, O in the small percentages. This is in good agreement with the previous research that there are presence of Sn, Se, and S in the SnS_{1-x}Se_x film [2]

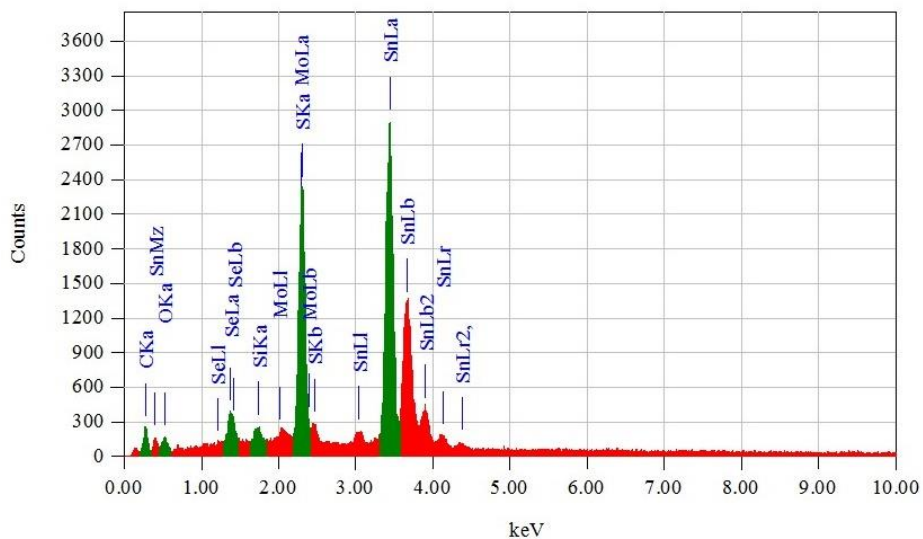


Figure 4. The EDX spectrum of SnSe_{0.2}S_{0.8} thin films at spacer of 15 cm

The detailed information of the elements contained in SnSe_{0.2}S_{0.8} thin films can be seen in Table 3. The presence of O element may be caused the oxidation process during preparation samples and the C element appeared is due to the heating process in high temperature.

Table 3. The EDX result for each element in SnSe_{0.2}S_{0.8} thin films ($d=15$ cm)

Element	keV	Mass %	Atom %
C	0.277	12.89	46.02
O	0.525	4.31	11.55
Si	1.739	0.65	0.99
S	2.307	10.64	14.24
Se	1.379	4.24	2.31
Mo	2.293	6.73	3.01
Sn	3.442	60.54	21.88

4. Conclusion

SnSe_{0.2}S_{0.8} thin films were successfully grown by evaporation techniques and characterized by XRD, SEM, and EDX. The crystallite size and strain contributions to line broadening were investigated by the Williamson-Hall method with Uniform Deformation Model. The increase of the spacer ($d= 10, 15, 25$ cm) causes the increase in the value of strain and crystallite size. SEM images show the homogeneity of grains distributions and proved the majority presence of Sn, S, and Se in the SnSe_{0.2}S_{0.8} thin films by EDX.

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