Sb_2Se_3 Thin-films for the next generation solar cells

4ª OFICINA DE INSTRUMENTAÇÃO E INOVAÇÃO

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INTRODUCTION

In recent years, antimony selenide (Sb_2Se_3) has emerged as a promising candidate for thin-film solar cells due its attractive optoelectronic properties with desirable band-gap (1-1.2 eV) [2]. Moreover, low cost of naturally abundant Sb and Se, high optical absorption coefficient of above 10^5 cm^{-1} in the visible region, stable chemical properties and long carrier lifetime makes Sb_2Se_3 a sophisticated absorber material for high power conversion efficiency photovoltaic device application [1]. In this work, four Sb_2Se_3 thin-films were grown at different substrate temperatures (room temperature (RT), 150°C, 250°C and 350°C) with the help of magnetron sputtering. The X-ray diffraction peaks ensure that the films are polycrystalline in nature. The topographic measurement using AFM demonstrates that there is an increase of average grain size as the substrate temperature increases. The XPS measurement provides an estimation of elemental quantification of Sb (57.8%) and Se (42.2%) and it shows that there is a loss of Se during the deposition.

MATERIALS AND METHODS:

Four Sb_2Se_3 thin-film samples were grown on Si(100) substrate with the help of AJA International Inc. sputtering system (shown in the Fig.1). The 99.99% pure Sb_2Se_3 target was sputtered with Ar ion at the RF power of 30W and the deposition pressure was 5 mTorr. The films were deposited at different substrate temperature (RT, 150°C, 250°C and 350°C) and their deposition time was fixed to 45 mins. The deposition rate (0.228 nm/s) was investigated with the help of X-ray reflectivity measurement. The average thickness of the samples were ~ 600 nm. The structural properties were studied by grazing incidence X-ray diffractometry (GIXRD) using a Panalytical X'Pert Pro diffractometer with Cu-Kα radiation (λ = 1.54056 Å). The chemical composition of the films was estimated using X-ray photoelectron spectroscopy (XPS) (SPECS-PHOIBOS 100/150) equipped with an Al Kα (1486.6 eV) X-ray source and a monochromator mirror with a Ag 3d5/2 resolution = 0.5 eV at the FWHM. All peaks fitting for the high resolution measurements for Sb 3d, Se 3p and C1s peaks was performed with the CASA-XPS software

RESULTS:

The XRD measurement in the range of 30-60° shown in Fig 2. The XRD peaks exhibits that as-deposited Sb_2Se_3 films are polycrystalline. The main peaks of Sb_2Se_3 phase are located at ~ 36.6°, 40.7°, 46.6° and 58.9° and their corresponding orientation are (112), (013), (312) and (214) respectively. The XPS spectra of Sb_2Se_3 films is shown in the Fig 3. All peaks in the spectrum were calibrated with respect to C1s (284.6 eV). The difference in the $3p_{3/2}$ and $3p_{1/2}$ levels for Se was ΔSe ($3p_{3/2}$ − $3p_{1/2}$) = 6eV and that for the 3d levels of Sb was ΔSb ($3d_{5/2}$−$3d_{3/2}$) = 9.84 eV. In the samples, the binding energies for the Se $3p_{3/2}$ and P $3p_{3/2}$ were 161 eV and 167 eV respectively, whereas binding energies of Sb for the $3d_{5/2}$ and $3d_{3/2}$ were 530 eV and 540 eV respectively. The elemental quantification determined from XPS spectra demonstrates that there is 57.8% Sb and 42.2% Se present in the films.

Fig. 1 –AJA international Inc. sputtering system

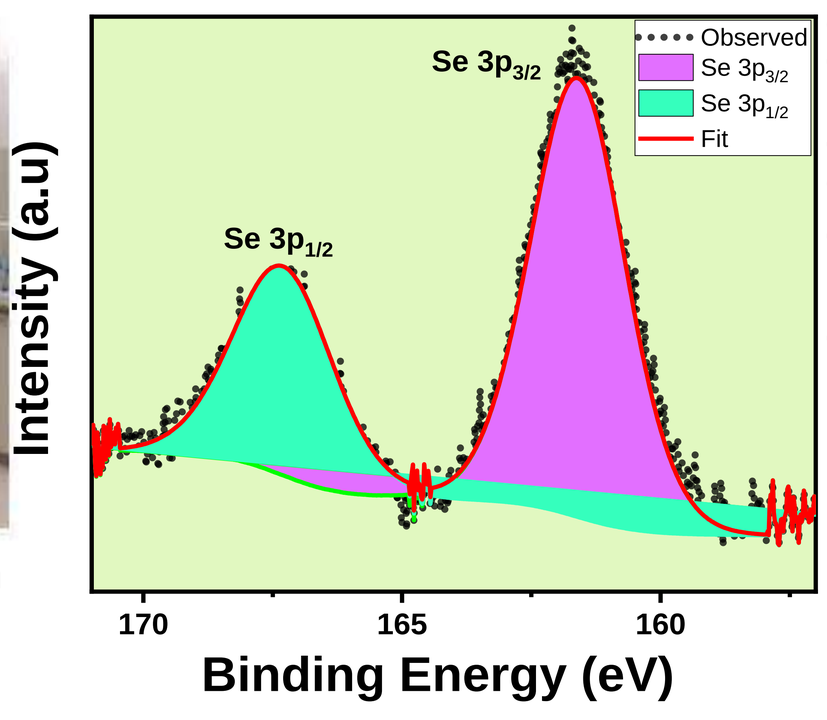

Fig.3-XPS spectra of Se 3p level of Sb_2Se_3 film deposited at 350°C substrate temperature

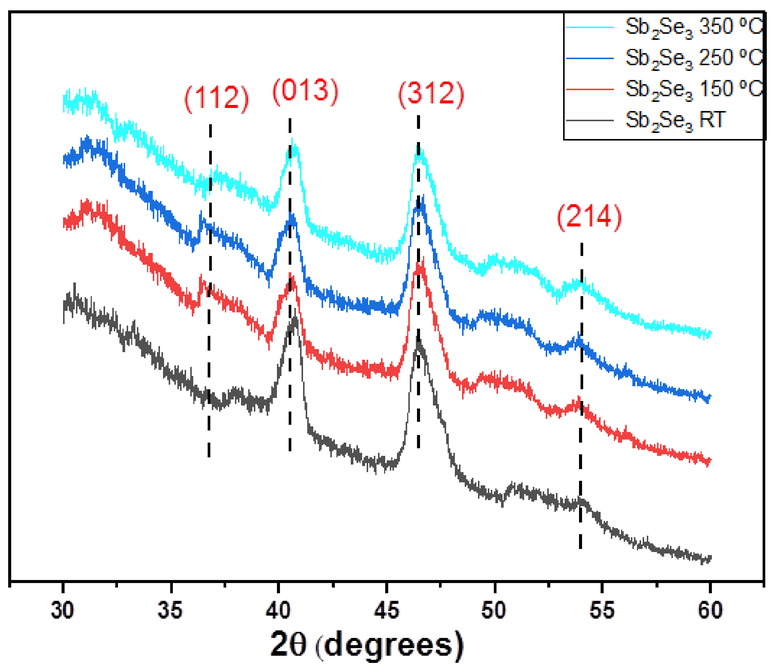

Fig.2- XRD spectra of Sb_2Se_3 films

CONCLUSIONS

- As-deposited Sb_2Se_3films are polycrystalline in nature
- Sb_2Se_3 phase is present in the films
- The different substrate temperature does not influence the crystalinity of the samples
- Elemental quantification obtained from XPS spectra exhibits that there is loss of Se during the deposition. The loss of Se may be caused by the higher vapor pressure of Se [3]

References:

[1] Wang et al. Nat. Energy **2**, 17046 (2017)

[2] Ghosh et al. Sol. Energy **211**, 613-621 (2020)

[3]Tang et al. Surface and coating Technology **360**, 68-72 (2019)