PREPARATION AND CHARACTERIZATION OF SbSeI THIN FILMS

Marc Dolcet Sadurni[1], Kristi Timmo[1], Valdek Mikli[1], Olga Volobujeva[1], Jüri Krustok[1], Maarja Grossberg-Kuusk[1], Marit Kauk-Kuusik[1]

[1]*Department of Materials and Environmental Technology, Tallinn University of Technology, Ehitajate tee 5, 19086 Tallinn, Estonia*
marc.dolcet@taltech.ee

Pnictogen chalcohalides consist of earth abundant, low-cost and low toxicity elements. Their crystals exhibit a pseudo-1D crystal structure and growth rate anisotropy, and when properly oriented, they enhance carrier transport and reduce charge carrier recombination [1]. Pnictogen chalcohalides-based solar cells are predicted to have excellent performance due to the presence of cations with a ns^2 electronic configuration that provides good defect tolerance (similar to Pb-perovskites) [2]. Among them, antimony selenoiodide (SbSeI) has received rising interest for different optoelectronic devices. It has indirect bandgap of 1.67 eV and SbSeI solar cells exhibited great stability as well as an efficiency of 4.1% [2].

In this work, SbSeI thin films were prepared through a two-step process. At first, Sb_2Se_3 thin films were deposited by magnetron sputtering and afterwards iodized isothermally in the sealed quartz ampoules in the SbI_3 atmosphere. The influence of annealing temperature, pressure and time on the morphology, composition, structural and optical properties of SbSeI thin films were studied. XRD, SEM, EDX, RT-Raman and RT-PL spectroscopy as characterization methods were used.

EDX and SEM results showed that the chemical composition and the morphology of the crystals of formed thin films depended strongly on the annealing pressure, temperature and time. SEM analysis showed that formed SbSeI thin films consist of single-crystal micro-columnar structures. The most homogeneous with stoichiometric composition of SbSeI were obtained by annealing the Sb_2Se_3 films in SbI_3 vapor at 250 °C for 5 min under 100 Torr of Ar pressure. XRD analysis revealed that the material has an orthorhombic lattice structure with space group Pnma 62 and lattice parameters a = 8.671204 Å, b = 4.118192 Å and c = 10.381914 Å. All the reflections belong to the SbSeI, with two main at 2θ angles of 29.4° (112) and 43.9° (020). Raman spectra showed main peaks at 95, 116, 137, 165, 184, 209, and 214 cm^{-1} that belong to SbSeI and confirm the XRD results. Room temperature PL of SbSeI revealed a broad asymmetric PL band with maximum at 1.67 eV.

References

1. A.M. Ganose, K.T. Butler, A. Walsh, D.O. Scanlon, J. Mater. Chem. A. 4 (2016) 2060–2068.
2. R. Nie, M. Hu, A.M. Risqi, Z. Li, S. Il Seok, Adv. Sci. 8 (2021) 1–8.

Euroopa Liit
Euroopa
Regionaalarengu Fond

Eesti
tuleviku heaks