# INVESTIGATION IF SBSEI THIN FILMS WITH OPEN AND CLOSED ANNEALING VARIATIONS

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Recently, antimony selenoiodide (SbSeI), one of the chalcohalide semiconductors that belongs to V-VI-VII class materials has been the subject of growing interest for applications, such as, X-ray and γ-ray detection, photocatalysis, solar cells, and in other optoelectronic devices. SbSeI enjoys additional benefits compared to other PV thin film systems, including the earth abundant and low toxicity chemical composition, high thermodynamic stability and large absorption coefficient (up to $10^5$ $cm^{-1}$). Although SbSeI has very promising properties, there are few studies where this material has been used as an absorber layer in solar cells and reported power conversion efficiency was low 4,1 % [1]. One of the key challenges in synthesizing SbSeI thin film absorbers for PV application, is its tendency to form porous needle-like structure [2].

Because of quasi-1-dimensional crystalline structure of SbSeI, it has a preferred growth direction along [001] axis resulting in rod-shaped grain growth. The goal of this study was to find synthesis approach that could allow to obtain continuous, uniform and compact SbSeI thin films morphology.

In this study we used a two-stage synthesis route where the first precursor layers were deposited and then followed by annealing step. SbSeI precursors films were deposited under vacuum by thermal evaporation method. Thin films deposition parameters, such as evaporation power, distance from source to substrate and source boat geometry were optimized for synthesis of compact, uniform, continuous precursor films. For the crystallization stage, annealing under $N_2$ atmosphere was performed with temperatures ranging from 150 $^oC$ up to 300 $^oC$ to achieve crystalline, compact SbSeI thin film with molar ratio near 1:1:1. Two annealing configurations were explored: a) open space and b) closed space. Structural properties of SbSeI thin films were characterized by XRD (θ-θ, Bragg-Brentano geometry), SEM and EDX methods.

In terms of precursor film homogeneity and uniformity in thickness, we found that optimal distance between source and sample was 5 cm. Also we found that precursor film composition was dependent on the evaporation power and under optimal conditions near-stoichiometric molar composition was obtained in open configuration, but at higher substrate temperatures SbSeI starts to decompose and $Sb_2Se_3$ phase is present. On contrary, annealing with closed configuration resulted in a stable SbSeI phase even up to 300 $^oC$. Using a two-stage synthesis route we were able to achieve uniform, compact and high crystalline quality SbSeI thin films.

[1] Nie, Riming, et al. "Efficient and stable antimony selenoiodide solar cells." Advanced Science 8.8 (2021): 2003172.
[2] Caño, Ivan, et al. "SbSeI and SbSeBr micro-columnar solar cells by a novel high pressure-based synthesis process." Journal of Materials Chemistry A 11.33 (2023): 17616-17627.