

SUMMARY

The initiatives in moving away from hydrocarbon-based energy supplies call for increasing capacities of sustainable energy sources and thus materials associated with them. Solar energy is one of the most important sources of low-carbon energy and both photovoltaic solar cells and solar-to-hydrogen strategies are among highly potential tools for green energy transition. The most advanced in the commercial sense, absorber materials beyond energy-inefficient silicon are utilizing toxic and scarce materials. Antimony selenide is an emerging semiconducting material with high potential due to low toxicity, cheap raw materials, relatively energy-efficient production and suitable properties.

Antimony (III) selenide as a photovoltaic absorber layer has a near-ideal optical band gap, absorption coefficient and relative dielectric constant, while non-toxic and relatively earth-abundant elemental composition defines a potential for industrial-scale application. Various deposition methods have been tested and used consistently to produce Sb_2Se_3 thin films, however, synthesis of high-quality material using them is a nontrivial task due to factors like relatively low decomposition temperature, ease of oxygen incorporation from solvents or atmosphere and complex defect chemistry of the material itself. As a result, the optoelectronic properties are unpredictable and can yield both p- and n-type semiconductors, often not reaching desired charged carrier concentrations. Thus, due to complex defect chemistry, the progress in high-quality Sb_2Se_3 material synthesis is limited by an inability to control the optoelectronic properties.

Doping is often addressed as a way to compensate for that effect, nevertheless, multiple attempts using conventional methods have shown no significant improvement in the ability to control electrical properties and have led to the formation of undesired phases or interferences with crystal structure. Cation exchange is a technique that proved effective in doping and transformation of nanocrystals, yet not explored enough on thin films.

In this work, silver ions were introduced into Sb_2Se_3 thin films by treatment in a glycerol solution containing only AgNO_3 or AgNO_3 combined with NaHCO_3 at 210 °C for 17 minutes. It was concluded that the silver incorporation rate depends on the choice of complexing agent and in the case of pure Ag source, a partial phase transformation to AgSbSe_2 and Sb_2Se_3 is inevitable.

Multiple chemicals were tested to suppress phase transition and incorporate Ar ions into the lattice, yet only NaHCO_3 successfully suppresses Ag ions and introduces dopants without a phase change. Silver incorporation at 1.5 at% using AgNO_3 in combination with NaHCO_3 was confirmed by TEM/EDX and the phase preservation was observed by XRD and Raman spectroscopy, while PL spectroscopy showed a drastic change in comparison to the pristine sample.