



# Yb-doped SnTe semimetal thin films deposited by thermal evaporation: Structural, electrical, and thermoelectric properties



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## ABSTRACT

Sn monochalcogenide and Yb-doped  $\text{Sn}_{1-x}\text{Yb}_x\text{Te}$  ( $0.0 \geq x \leq 0.1$ ) semimetals, which are known for their usefulness as efficient thermoelectric (TE) materials, were prepared by solid-state microwave technique. Polycrystalline thin films of  $\text{Sn}_{1-x}\text{Yb}_x\text{Te}$  were deposited onto clean glass substrates by using vacuum evaporation technique at  $10^{-6}$  bar. The structures of the polycrystalline thin films were examined by X-ray diffraction patterns. A rock salt structure was observed. Grain size increased with increasing Yb content but not according to a sequence. The morphology of the nanosheet structures for these thin films was determined by field emission scanning electron microscopy. TE properties were measured at a temperature range of 298–523 K. The carrier concentrations of the films were determined by Hall effect measurements at 300 K.

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## 1. Introduction

SnTe has recently received considerable attention for its potential applications as a thermoelectric (TE) energy converter and electronic device [1,2]. For mid-temperature power generation at 800 K, materials based on group-IV telluride are typically used, such as SnTe, PbTe,  $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$ ,

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and  $\text{AgPb}_m\text{SbTe}_{2+m}$  [3,4]. An efficient method to increase the Seebeck coefficient ( $S$ ) and the power factor ( $S^2\sigma$ ) of a homogeneous semiconductor is proposed in [5,6], which verifies the possibility of transforming bipolar semiconductor films. An alternative to doping can be conducted to obtain practically monopolar semiconductors. The effectiveness of using such semiconductors is determined by the possibility of obtaining high values of TE characteristics, such as  $S$  and  $S^2\sigma$  [7,8]. Electrical conductivity ( $\sigma$ ) is mainly determined by the electronic band structure, which can be improved through appropriate chemical doping. Phonon transportation is mainly responsible for the thermal conductivity of semiconductor-based TE materials [9,10]. The TE characteristics of semiconductors depend on the position of the Fermi level; the concentration, mobility, and effective mass of the charge carriers; the mechanisms of their scattering that simultaneously depend on temperature; and the preparation technique [11,12]. Carrier concentration ( $n$ ) can be changed by doping in several rare earth elements. Doping can strongly affect the transport properties of TE materials via the formation of the following mechanisms: enhanced electron states near the Fermi level, local defects that result in additional carrier scattering, and additional carrier scattering from localized magnetic moments (to attract the density of states of electrons and phonons). These mechanisms tune the band gap of TE materials to make them suitable for high-performance TE devices [13,14]. Most of these compounds are grown by different molecular beam epitaxy methods that employ expensive equipment for vacuum deposition, including sputtering, reactive evaporation, chemical vapor deposition, and solid-state reaction techniques. [15–19]. The TE materials of  $\text{Sn}_{1-x}\text{Eu}_x\text{Te}$ , which are prepared by heating mixtures above the melting point of the constituent elements through the well-known Bridgman method, have been examined recently [20]. In the current study, ternary SnTe semiconductor materials are prepared by doping with Yb using the solid-state microwave synthesis technique at a temperature range of 1204–1252 K and a growth time of 25 min. The fundamental properties of SnTe alloys are investigated by analyzing their structural and electrical characterizations for thin films. Rare earth impurity Yb forms resonance electron states near the Fermi level and affects electronic transport properties significantly, particularly  $S$ . Therefore,  $\sigma$  and  $S$  are enhanced with an increase in the Yb mole fraction of  $x = 0.0$ – $0.1$ . Accordingly,  $S^2\sigma$  increases with an increase in Yb concentration in dramatically doped thin films.

## 2. Experimental procedure

Solid-state microwave synthesis was conducted to prepare the ternary polycrystalline ingots of  $\text{Sn}_{1-x}\text{Yb}_x\text{Te}$  alloys. For each high-purity Sn, Te, and Yb powders (Sn and Te,  $\geq 99.999\%$ , 100 meshes; Yb,  $\geq 99.9\%$ , 157  $\mu\text{m}$ ), 2 g were obtained by weighing using an electronic balance based on the stoichiometric ratio  $1:(1-x):x$ . The mixture was transferred into an agate mortar and pestle, ground for 20 min, placed in a quartz ampoule, and sealed after evacuation at  $1.6 \times 10^{-5}$  mbar. The ampoule was exposed to microwave energy operating at 2.45 GHz for 25 min, with a maximum power of 800 W inside a cavity microwave oven (MS2147C 800 W). The reaction time was recorded, and the mixture was shaken every 5 min. During the timed reaction, the  $\text{Sn}_{1-x}\text{Yb}_x\text{Te}$  compound flashed bright whitish-green when the configuration of the composite was completed [9,21]. Thin films of ternary  $\text{Sn}_{1-x}\text{Yb}_x\text{Te}$  were then deposited onto clean glass substrates by using the thermal evaporation technique in a vacuum at  $6.4 \times 10^{-6}$  mbar by an Alcatel-101 with a Ta boat to obtain thin films with a thickness of  $174 \pm 6$  nm measured by using an optical reflectometer (Filmetrics F20, USA). X-ray diffraction (XRD) patterns of undoped and Yb-doped SnTe thin films were recorded by Cu K $\alpha$  ( $\lambda = 0.154056$  nm) radiation with  $2\theta$  within the range of  $10$ – $90^\circ$  (PANalytical X'Pert PRO MRD PW3040). The surface morphology of the thin films was examined through field emission scanning electron microscopy (FESEM, Leo-Supra 50VP) and atomic force microscope (AFM, Model Dimension EDGE, BRUKER). The electrical properties ( $S$  and  $\sigma$ ) of the films were measured at a temperature range of 298–523 K. The two ends of the films were coated with Al by thermal evaporation in a vacuum using a vacuum coater unit Auto 306.  $n$  and majority carrier type were measured by the Hall effect using the van der Paw method at 300 K. Measurement was performed by applying a vertical constant magnetic field of 1 T to the thin films using Lake Shore DEC-637.

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