



Effect of Structural Changes on the Mechanical Properties of Sintered Films

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Abstract

Polycrystalline films of tin telluride were prepared by sintering technique. The structural investigation of the films with different thicknesses enables to determine lattice parameter, crystallite size and strain existing in the films. The XRD traces showed that strain was tensile in nature. The crystallite size increases with thickness while strain decreases. Higher the value of tensile strain, larger is the lattice constant. The optical energy gap shows a descending nature with increasing strain and so with the lattice constant. Such an attempt made to delve into interdependence of basic physical quantities helps to explore the properties of SnTe and utilize it as an alternative to heavy metal chalcogenides in various technological applications.

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Keywords

Sintering, Lattice parameters, crystallite size and strain

Introduction

In recent years, use of heavy metals especially lead, cadmium, and mercury in semiconducting industry, paints and coatings has been restricted throughout the world [1], on account of their detrimental effects on health. In order to replace such metals from various semiconductor and optoelectronic applications, it becomes quite necessary to search for their alternatives and look at possible compounds having similar properties with sufficient stability.

To solve the purpose, tin based compounds have emerged as potential materials for their wide application in industry and research [2-6]. Tin chalcogenides SnS, SnSe and SnTe offer a group of promising materials for solar applications and optoelectronics in far infra-red region of the spectrum as well as for thermo electric devices at medium high temperature [7].

The technological interest in polycrystalline based devices is caused mainly due to their low production cost which makes them suitable for large scale applications. SnTe belongs to a class of self doping compounds i.e. metal chalcogenides. It is known to be a p-type semiconductor with strong self compensation of p-type conduction. Different workers prepared SnTe films by vacuum based expensive techniques [8-10] but the sintering technique employed here to prepare SnTe films is simple and commercially viable. The ease of preparation method and its cost effectiveness has made it apt for large area applications. The present paper reports the results of physical properties of SnTe films particularly structural and mechanical. From the XRD studies, interplanar spacing, lattice parameter, crystallite size and strain have been determined for the sintered films of different thickness and an attempt to establish an explicit co-relation between various quantities has been made.

Experimental Details:

SnTe films were deposited by conventional screen printing followed by a sintering technique. The starting material SnTe was prepared by mechanical alloying. The constituent elements (Sn and Te) of high purity (99.99%) were taken in stoichiometric ratio and mixed properly in mortar and pestle for 10 minutes at room temperature with continuously shaking to maintain homogeneity of the samples. Stannic chloride $\text{SnCl}_4 \cdot 2\text{H}_2\text{O}$ as added as adhesive in appropriate proportion and ethylene glycol was added as binder. The paste thus prepared was screen printed onto ultra clean glass-substrate, which has been cleaned by HCl, soap solution, embryo powder and finally washed with distilled water. The samples thus prepared were dried at 120°C for 1 hour in open air. The reason of drying the samples at lower temperature was to avoid the cracks in the sample. The films were sintered at a temperature of 200°C for 10 minutes in a temperature controlled furnace in air atmosphere. For good stability of the films it is necessary that stannic chloride and ethylene glycol should be removed from the samples. Three sets of samples with different thicknesses were prepared under the same experimental conditions to examine the reproducibility of the samples. The thickness of the samples was measured by Xi-100 non contact optical profiler. The prepared sintered films were characterized by X-Ray diffraction study using Bruker AXS D8 Erz Nr 7K P2025 Karlsruhe (Germany) diffractometer employing $\text{CuK}\alpha$ radiation ($\lambda = 1.5405\text{\AA}$) in the range 5° - 90° at the speed of $2^\circ/\text{min}$. The absorption spectra of the sintered sample are taken at room temperature with the help of Varian Cary 5000 UV-VIS-NIR spectrophotometer.

Results and Discussion

X ray diffraction is a powerful tool to obtain information about crystal structure, nature of crystallite material etc. XRD pattern of SnTe films prepared on glass substrate are shown in (fig 1). The XRD pattern reveals that the deposited

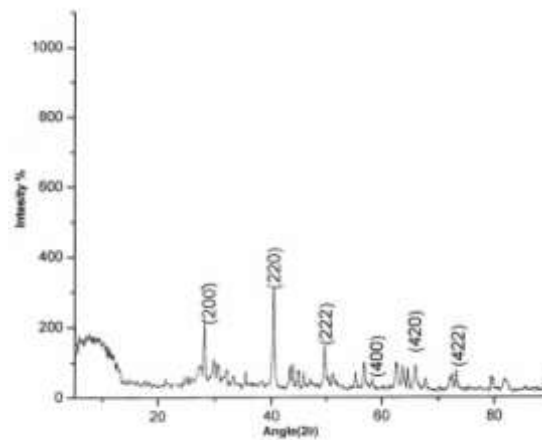


Fig 1. XRD pattern of SnTe film thickness 235µm

films are polycrystalline in nature [11]. Different XRD peaks were indexed and corresponding values of interplanar spacing 'd' were calculated from Bragg's relation $2d_{hkl} \sin\theta = n\lambda$ (here $n=1$, $\lambda=1.5405 \text{ \AA}$) and θ values were taken from peaks of XRD pattern. The 'd' values were in good agreement with the ASTM data. Using full width half maximum (FWHM) data and Debye Scherrer formula, the crystallite size, lattice constant and strain were calculated for SnTe films synthesized for different thickness values.

$$D = 0.94 \lambda / \beta \cos\theta$$

where, D is the grain size (in nm), β is the Full Width at Half Maximum (FWHM) of the particular peak, θ (rad) is the Bragg's angle and λ is the wave-length of X-Ray.

Displacement and broadening of X-Ray peaks provide information about deformation and crystallite size of the films. The broadening of the diffraction peaks is usually caused by small crystallite size as well as extension of micro stress in the films. The term micro stress is used to indicate their variation from one grain to another on microscopic scale. In fact stress remained in the films on removing all the external forces, causes important effects on the physical properties of the materials. The stress remained in the films can be determined from the strain by multiplying the average

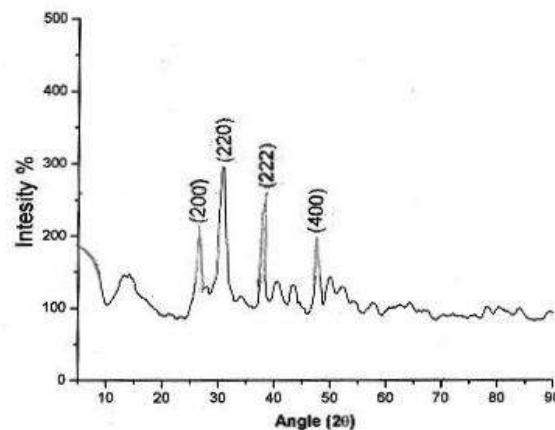


Fig 2. XRD pattern of SnTe film thickness 345µm

strain $\Delta d/d$ by elastic constant of the material. Our samples have undergone through investigation with respect to strain being more rudimental property. The strain in the films was determined using the relation $\Delta d/d = (d_0 - d_{ASTM})/d_0$, where 'd₀' is the d spacing measured for the films and d_{ASTM} is the corresponding 'd' spacing of single crystal as reported in a ASTM card.

The displacement of the peak to the left and increased 'd' spacing manifests tensile stress (fig 2) while displacement to the right and decrease in 'd' spacing implies compressive stress acting on the film. The tensile stress is

caused by the vacancies [12]. In the present investigation the tensile stress may be addressed to Sn vacancies

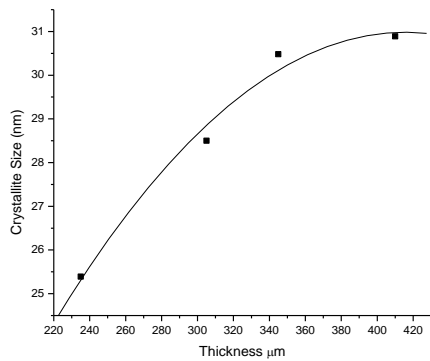


Fig 3. Variation of crystallite size with thickness of SnTe sintered films.

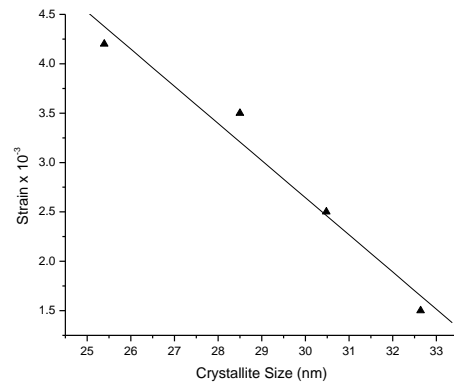


Fig 4. Variation of strain with crystallite size of SnTe sintered films.

which lead to implantation of acceptor levels within forbidden gap having a tendency to trap the electrons from valence band resulting in a stretching force on them. The strain observed in the films decreases with crystallite size as shown in (fig 3) and the enhancement in crystallite size with thickness can be observed from (fig 4) upto $\approx 300\mu\text{m}$. If further thickness is increased the crystallite size gives the indication being thickness independent. The strain observed in the films also affected the lattice constant of the material. Fig 5 represents the effect of strain on lattice constant. The lattice constant is enhanced due to existence of tensile stress in the films.

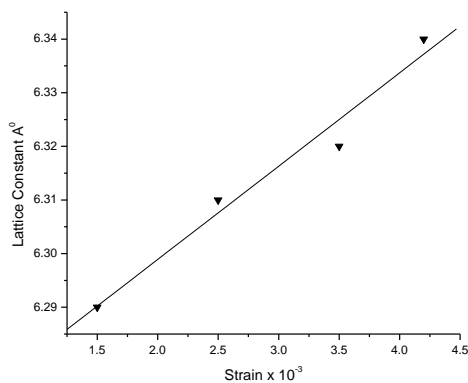


Fig 5. Variation of lattice constant with strain of SnTe sintered films.

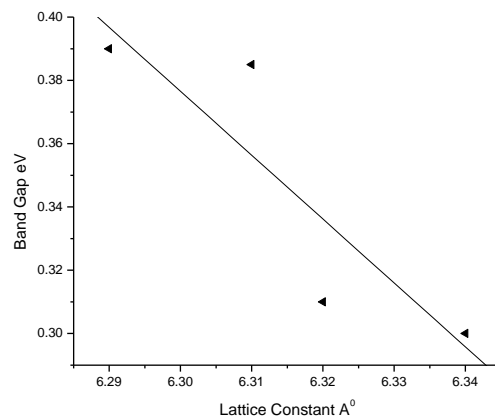


Fig 6. Variation of Band gap with lattice constant of SnTe sintered films.

To determine the energy band gap (E_g) in terms of absorption co-efficient is given by Tauc's relation [13].

$$\alpha h\nu = A (h\nu - E_g)^n$$

where α is absorption coefficient, $h\nu$ is photon energy, A is constant, E_g is the band gap and $n = \frac{1}{2}$ for allowed band to band (direct) transitions and 2 for allowed indirect transitions. The energy band gap of the SnTe films also vary with lattice constant which can be seen from fig6. The narrowing trend in the forbidden energy gap with increased strain values may be associated to the implantation of acceptor levels which in turn causes effective forbidden energy gap to decrease.

Conclusion

Tin telluride films were screen printed on glass substrates by screen printing following the sintering and their structural and mechanical properties were examined. The crystallite size of the samples was found to depend on thickness and the strain in the films showed its dependence on crystallite size. The strain also causes the lattice constant to expand. The enhanced lattice constant resulted in reduced energy band gap. Such explicit interdependence of various physical quantities in useful in extending the practicability of SnTe material in near IR and mid IR optical, photovoltaic and thermoelectric devices. The present investigations would capacitate to use environment friendly tin-chalcogenides in various technological applications and substitute for health hazardous lead and cadmium chalcogenides from semiconductor industries.



(N.B. : The Figures 1 to 6 have also been reattached later for higher resolution view in Jpeg Format.)

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