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Optical Studies of $Se_{80}In_5Te_{10}Sb_5$ Nano Chalcogenide Thin Films of Different Thickness

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Abstract

This present study explores the effect of film thickness on the optical parameters of $Se_{80}In_5Te_{10}Sb_5$ nano-scale chalcogenide thin films deposited on glass/Si wafer substrates using the thermal evaporation technique under a vacuum of 10^{-6} Torr. The amorphous structure of the films was verified by High Resolution X-ray characterization, and their surface morphologies were subsequently investigated using FESEM. The optical constants of the thin films were evaluated from absorption spectra as a function of photon energy within the 400–1100 nm wavelength range. Chalcogenide glasses exhibit strong thickness-dependent optical properties such as changes in optical band gap, refractive index, and absorption coefficient. Experimental outcomes indicate that with the increase in film thickness, the optical band gap tends to decrease and other optical parameters differ methodically because of quantum confinement and structural disorder effects. The outcomes play a key role in enabling the rational design of chalcogenide films for advanced photonic and optoelectronic devices.

Keywords: *Thin film, XRD, FESEM, Optical band gap.*

1. Introduction

In recent decades, widespread theoretical and experimental researches have exposed the excellent properties of chalcogenide materials and emphasized their vital role in advancement of emergent technologies. Chalcogenides are compounds that contain at least one chalcogen element, namely sulfur (S), selenium (Se), or tellurium (Te). Prompt development in multimedia technologies has been driven by growths in computing power and data storage density, along with the developing demand for rewritable storage media. Among the numerous material systems discovered, chalcogenide-based phase-change (PC) materials have arose as some of the most capable candidates for rewritable data storage usage [1], [2]. Their superficial and reversible amorphous–crystalline phase switching makes them predominantly appropriate for information storage technologies. Chalcogenide thin films have therefore fascinated substantial consideration and have been methodically studied over the past several decades. Owing to their exclusive physical and optical properties, they remain a major focus of both experimental and theoretical investigations. These materials are extensively recognized as favorable platforms for diverse photonic applications, including ultrafast optical switching, frequency conversion, optical amplification, infrared lasers, phase-change memory devices, and infrared-transmitting optical fibers [3], [4], [5], [6], [7]. Optical storage based on the amorphous–crystalline phase transition exploits the pronounced changes in optical reflectivity and absorption induced in certain semiconductor–semimetal thin films upon thermal or laser treatment. To further explore application potential and enhance device performance, continuous efforts have been devoted to investigating the optical, structural, and thermal properties of ternary and quaternary chalcogenide glasses [8], [9], [10]. The optical properties of chalcogenide glasses are strongly dependent on structural parameters, especially thickness of the nano-thin film. Thickness can alter quantum confinement effects, defect densities, and light–matter interactions at the nanoscale, making comprehensive thickness-dependent optical studies essential for device optimization.

Many researchers have explored about the thickness dependency of the optical properties of chalcogenide glasses and tried to optimize the thickness of the chalcogenide thin film for the device applicability purposes. Sharma and Katyal [11] have studied the thickness dependency of optical properties of the thin films of Ge-Se-Te chalcogenide glasses and found that optical band gap was decreases with the thickness of the films. Solieman et al. [12] have been explored thickness dependence of the optical properties of amorphous Ge30Se70 thin films. Nidhi et al. [13] has been done the optical studied of Te-Se-Ge-Sb glassy thin films and found the variation in their optical and structural properties with film thickness. Tripathi et al. [14] have been done the optical and electrical studies of Se-In-Bi nano chalcogenide thin films and reported the variation in properties with thickness. Thickness dependence of the optical properties of amorphous As-Ge-S thin films has been studied by Todorov et al. [15]. The correlation between structural and optical properties and thickness of textured Cd-Se thin film has been explored by Zubair et al. [16]. Influence of thickness and annealing on optical constants of Se-Te-Sb chalcogenide thin films has been studied by Abdel Rahim et al. [17].

Keeping in view the above research works and their optimistic outcomes, we have decided to study the variation in optical constants of $Se_{80}In_5Te_{10}Sb_5$ chalcogenide thin films with thickness. Selenium (Se) has been chosen because of its appropriateness for phase-change memory (PCM) devices based on its reversible phase-change properties [18]. However, these materials suffer from aging effects, poor stability, and high sensitivity which can be modified by incorporating a proper metallic additive, such as indium, into selenium. Indium-doped selenium has applications in gas sensors, thermoelectric materials, and solar cells [19]. Furthermore, tellurium has been added to the Se–In alloy to enhance its crystallinity corrosion resistance [20]. Metallic doping in chalcogenides modifies the average coordination number and induces structural changes in the glassy matrix, leading to flexible, intermediate, and rigid phases. Sb has been incorporated into the ternary

Se–In–Te glassy alloy, which enhances the glass-forming region and introduces configurational as well as compositional disorder in the glassy system [21]. The aim of the present work is to study the thickness-dependent optical properties of $Se_{80}In_5Te_{10}Sb_5$ chalcogenide thin films for phase-change memory device applications.

Experimental:

The melt-quenching technique was employed for the synthesis of $Se_{80}In_5Te_{10}Sb_5$ chalcogenide glass using 99.999% pure constituent elements. The materials were weighed according to their atomic percentages and sealed in a quartz ampoule under high vacuum. The evacuated and sealed ampoule was then placed in a temperature-controlled furnace, where the temperature was increased in four steps: initially at 673 K for 2 h, followed by 873 K for 2 h, 973 K for 3 h, and finally 1023 K for 4 h. During heating, the ampoule was frequently shaken to ensure homogeneity. Rapid quenching in an ice–water bath was subsequently carried out to obtain the glassy material. The glassy and amorphous nature of the prepared sample was confirmed by DSC measurements. Nano thin films of $Se_{80}In_5Te_{10}Sb_5$ with thicknesses of 20 nm, 40 nm, and 60 nm were deposited onto glass and Si wafer substrates using an Edwards Coating Unit E-306 operated at a base pressure of 10^{-6} Torr and a deposition rate of 4 nm s^{-1}. Structural analysis of the as-deposited nano thin films was performed using a Rigaku Ultima IV X-ray diffractometer. The surface morphology of all films was examined using a field-emission scanning electron microscope (FESEM) (QUANT FEG 450, Amsterdam, Netherlands). Optical absorption measurements were carried out using a UV–Vis–NIR spectrophotometer (JASCO V-500) in the wavelength range of 400–1100 nm.

Result and Discussion:

The glassy and amorphous nature of the synthesized $Se_{80}In_5Te_{10}Sb_5$ material was confirmed by a non-isothermal differential scanning calorimetry (DSC) scan carried out at 25 K min^{-1} heating rate (Fig. 1). The observed endothermic peak corresponds to the glass transition of the sample, as the glass transition is a relaxation process that involves heat absorption. The exothermic peak is associated with the crystallization of the material. The presence of distinct glass transition (T_g) and crystallization (T_c) peaks confirms the glassy state of the sample. The T_g and T_c values were found to be 342 K and 391 K, respectively.

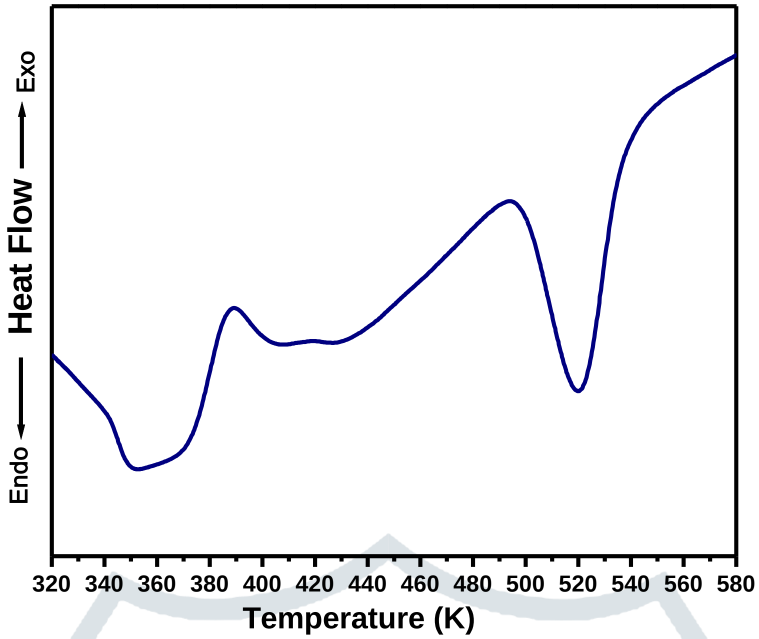

Fig. 1: DSC Thermogram of $Se_{80}In_5Te_{10}Sb_5$ Chalcogenide Glass

High-resolution X-ray diffraction (HRXRD) with Cu Kα₁ radiation (λ = 1.5406 Å) was employed to analyze the structural evolution of the $Se_{80}In_5Te_{10}Sb_5$ nano thin films of different thickness. The measurements were conducted at 40 kV and 30 mA with a step size of 0.05°, a counting time of 2.5 s, and a 2θ scan range of 10°–70°. The diffraction patterns shown in Fig. 2 has no any sharp peak which reveals that the as-prepared nano-films are amorphous in nature,

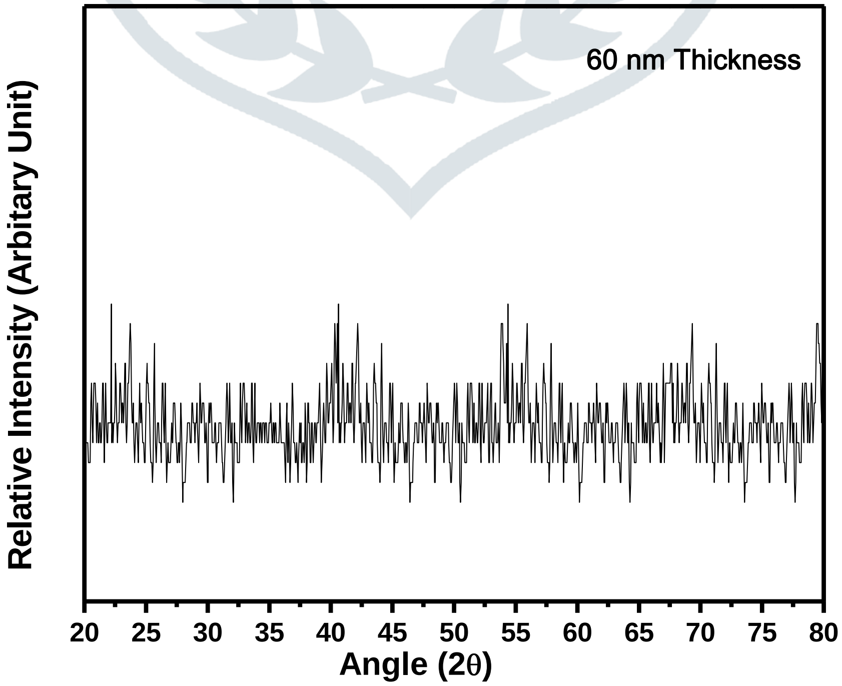

Fig. 2: HRXRD Diffraction Pattern of $Se_{80}In_5Te_{10}Sb_5$ nano thin Film

The surface morphology of the as-deposited $Se_{80}In_5Te_{10}Sb_5$ nano thin films of different thickness deposited on Si (100) substrates was examined by using field-emission scanning electron microscopy (FESEM). The FESEM analyses were done at an accelerating voltage of 20 kV with working distance 1 cm. Fig. 3 show the FESEM images of as-deposited $Se_{80}In_5Te_{10}Sb_5$ nano thin films. FESEM observations validate a noticeable thickness-dependent advancement in the surface morphology of the nano-chalcogenide thin films. The film with a thickness of 20 nm exhibits discontinuous coverage with isolated nano-islands and considerable surface porosity, revealing the early nucleation growth. As the thickness increases to 40 nm, these islands increasingly merge to form a more continuous granular network, followed by a reduction in void density and an increase in grain size. Further increasing the thickness to 60 nm yields a dense and compact surface with well-developed nanograins and minimal surface defects. This morphological transformation can be attributed to improved mobility and the extended deposition duration, which facilitate grain growth and film densification [22], [23].

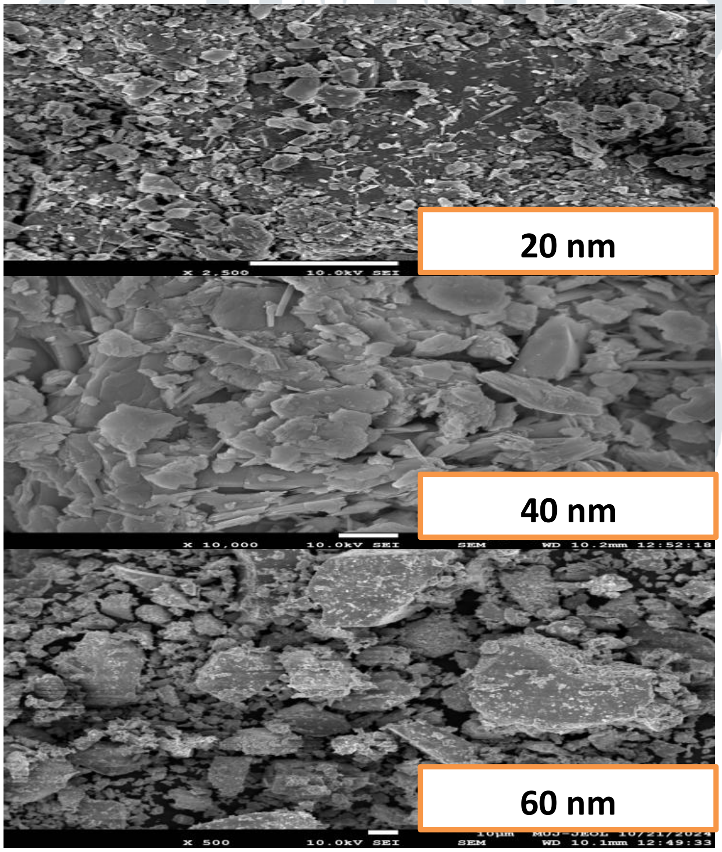

Fig. 3: FESEM Images of As-deposited $Se_{80}In_5Te_{10}Sb_5$ Nano Thin Films

A JASCO spectrophotometer with a photometric accuracy of 0.004 was used for the optical absorption measurement of the as-deposited $Se_{80}In_5Te_{10}Sb_5$ nano-thin films of different thickness. Absorbance is the amount of incident radiation absorbed by the sample under definite experimental conditions. Optical characterization of all the $Se_{80}In_5Te_{10}Sb_5$ nano-chalcogenide thin films was carried out using recorded absorbance data over the wavelength span 400–1100 nm. The absorption coefficient (α) was evaluated by the following relation [24], [25]:

$$\alpha = \text{Optical Absorbance/Thickness of the film} \quad (1)$$

The variation of the absorption coefficient (α) with photon energy (hν) for the $Se_{80}In_5Te_{10}Sb_5$ nano-chalcogenide thin films is presented in Fig. 4.

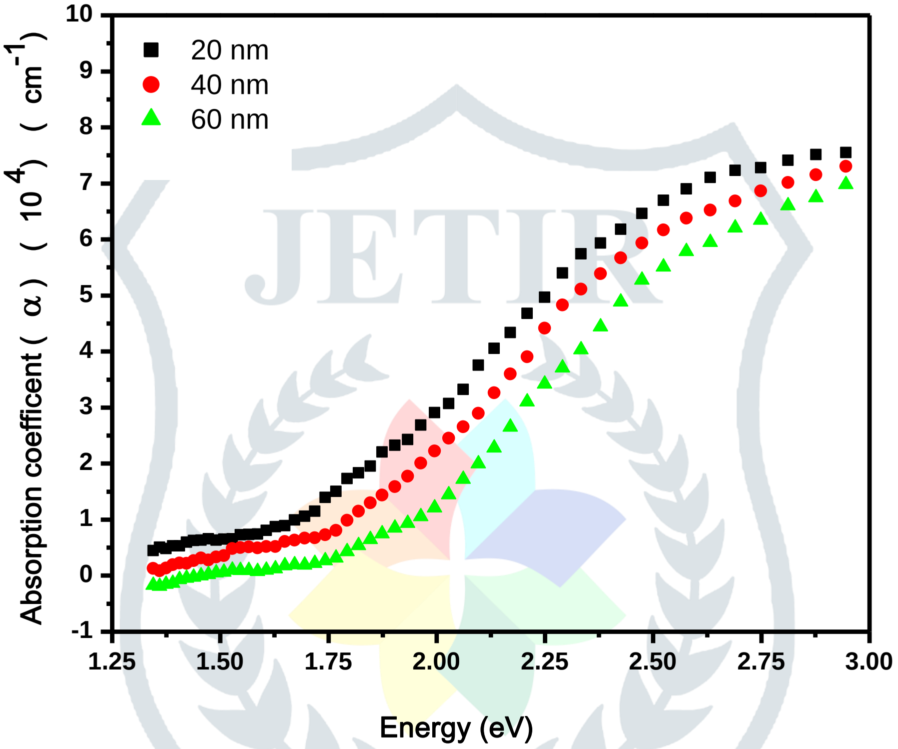

Fig. 4: The plot of the absorption coefficient (α) and photon energy (hν) for the $Se_{80}In_5Te_{10}Sb_5$ nano-chalcogenide thin films

It is evident from Fig. 4 that α increases with increasing photon energy, consistent with previously reported observations [26], [27] . The absorption coefficient (α) of nano-chalcogenide thin films also exhibits a clear dependency on film thickness. Thinner films show comparatively lower α values due to discontinuous coverage and higher surface porosity, which reduce the effective interaction between incident radiation and the absorbing medium. The values of the absorption coefficient at 690 nm for different thickness films are summarized in Table 1.

For most chalcogenide glasses, the relationship between the absorption coefficient (α), photon energy (hν), and optical band gap (Eg) follows Tauc's relation [28], [29]:

$$(\alpha h\nu)^n = A\,(h\nu - E_g) \qquad (4)$$

where A is a constant, E_g is the optical band gap, and n is an exponent whose value (2, 1/2, 2/3, or 1/3) depends on the nature of the optical transition [30]. For $Se_{80}In_5Te_{10}Sb_5$ nano-chalcogenide thin films, the best linear fit was obtained for $n = 1/2$, indicating an indirect allowed electronic transition [31]. Accordingly, plots of $(\alpha h\nu)^{1/2}$ as a function of photon energy ($h\nu$) were constructed, as shown in Fig. 5.

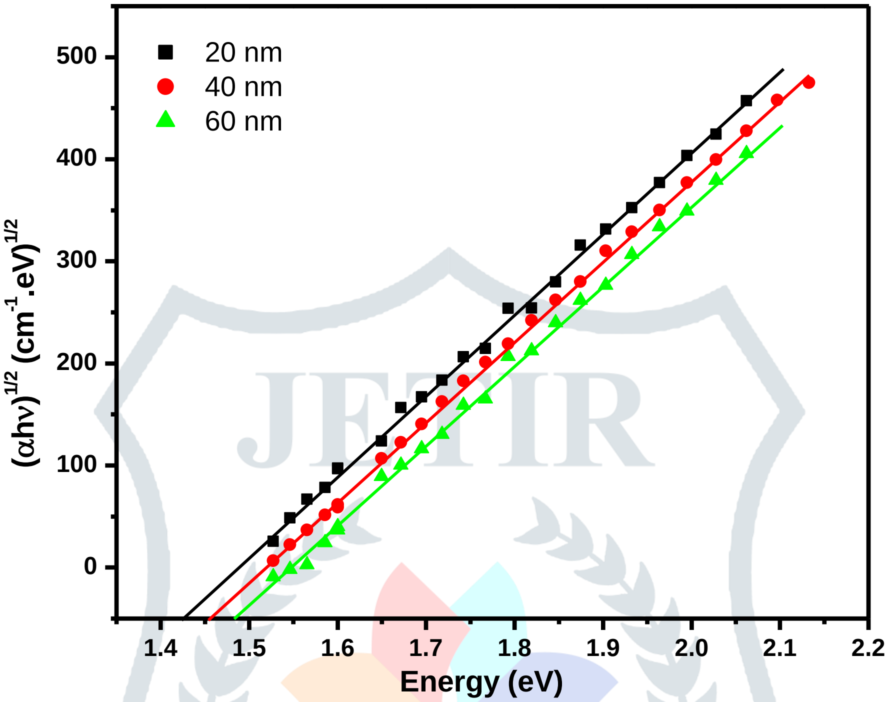

Fig. 5: The plots of $(\alpha h\nu)^{1/2}$ and photon energy ($h\nu$) for $Se_{80}In_5Te_{10}Sb_5$ nano-chalcogenide thin films

The optical band gap values were determined by extrapolating the linear portions of these plots to the energy axis, and the extracted E_g values are listed in Table 1. It is evident from Table 1 that the optical band gap decreases with increasing film thickness, in agreement with trends reported in earlier studies [32], [33]. This variation in optical band gap can be attributed to improved film continuity, reduced porosity, and a higher density of absorbing centers in thicker nano-chalcogenide layers [34], [35].

Table-1

Optical parameters of $Se_{80}In_5Te_{10}Sb_5$ nano-chalcogenide thin films of different thickness

Optical constants	*20 nm Thickness*	*40 nm Thickness*	*60 nm Thickness*
***Absorption coefficient (α) (10^4) (cm^{-1})* at 690 nm**	1.66	0.88	0.40
Optical Band Gap (E_g)(eV)	1.42	1.45	1.50

4. Conclusion

In this research work, we have analyzed the thickness effect on the optical properties of $Se_{80}In_5Te_{10}Sb_5$ nano-chalcogenide thin films. These amorphous structures of deposited films were confirmed by High Resolution X-ray diffraction and surface morphology of all films were examined by FESEM. The absorption coefficient and optical band gap were found to be strongly thickness dependent. These dependencies are mainly governed by the quantum size confinement effect, defect states and film structure. Such understandings enable the tunability of nano chalcogenide thin films for infrared optics, photovoltaics, and photonic devices.

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