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Thickness and optical constants calculation for chalcogenide-alkali metal $Se_{80}Te_8(NaCl)_{12}$ thin film

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ABSTRACT

Chalcogenide-alkali metal semiconducting thin films of four different thicknesses of $Se_{80}Te_8(NaCl)_{12}$ are deposited from bulk by thermal evaporation technique. The crystallinity of the film improves with increasing of thickness as indicated by the recorded X-ray diffraction patterns. The transmission and reflection spectra are measured in the wavelength range of the incident photons from 250 to 2500 nm. The thickness and optical constants of the films are calculated based on Swanepeol method using the interference patterns appeared in the transmission spectra. It is found that the films have absorption mechanism which is an indirect allowed transition. The effect of the film thickness on the refractive index and the high-frequency dielectric constant are studied. With increasing the film thickness, both the absorption coefficient and high-frequency dielectric constant increase while the single-oscillator energy, optical band gap and extinction coefficient decrease.

1. Introduction

Chalcogenide material films are the subject of optical measurement studies because of their optical properties for instance high transparence in visible and infrared regions [1]. They are apposite fabric for optical memory, disks, elements and sensors [2–6]. Chalcogenide films of selenium-tellurium have been used in fabrication of technological optoelectronic devises [6,7]. The use of these chalcogenides as optical materials in device applications is built in the values of their optical constants such as optical band gap, refractive index and extinction coefficient which are the most significant factors in thin films. Incorporation alkali metal like sodium in a chalcogenide matrix has a great effect for photovoltaic properties by increasing the fill-factor and hole density [8]. The addition of sodium also enhances the power conversion efficiency of solar cell [9,10]. The effect of the film thickness is considered as a probe tool to optimize the optical properties of thin films as the thickness affects the optical transmission and reflection spectra [11–13].

This work reports the calculation of the thickness and optical constants of deposited chalcogenide-alkali metal $Se_{80}Te_8(NaCl)_{12}$ thin film. We also give insight into the dependence of optical constants on the film thickness and analyzing the dispersion of the refractive index using the single oscillator model. According to literatures, this work is belonging to few number of papers concerning the optical properties of chalcogenide-alkali metal thin films.

2. Experimental

The bulk $Se_{80}Te_8(NaCl)_{12}$ chalcogenides are prepared using the melt-quench technique by using high purity (99.99%) of Se and Te elements and NaCl salt (Aldirch Co., UK). The complete description of bulk sample preparation was discussed in our pervious works [14,15]. Thin films of target thicknesses of 470, 560, 650 and 750 nm were prepared by thermal evaporation of the $Se_{80}Te_8(NaCl)_{12}$ bulk at 10^{-5} Torr using an Edwards E-306 coating system. The evaporation rate as well as the film thickness is controlled by using a quartz crystal monitor FTM5.

An X-Ray Diffractometer (Philips, PW 1710) was used to record the X-ray diffraction patterns for the deposited thin films. The transmittance (T) and reflectance (R) are measured using a double-beam spectrophotometer (Shimadzu UV-2101-Japan).

3. Results and Discussion

3.1. X-ray Diffraction

The X-ray diffractions of the $Se_{80}Te_8(NaCl)_{12}$ with four different film thicknesses (470, 560, 650 and 752 nm) are shown in Fig. 1. The ascent of the thickness is initially estimated from the weight of the evaporated bulk material by using a quartz crystal monitor FTM5. The mentioned accurate value of the thickness is then calculated as discussed herein after. For all films, Fig. 1 shows a broad hump in the range of 2θ between 17° and 30° indicating the amorphous content. Each film exhibits a single diffraction peak around at $2\theta = 31.40°$ indicating the material film is partially crystallized. The observed inter-planar spacing (d_{hkl}) of this peak is equal to 2.85 Å. The corresponding phase can be identified

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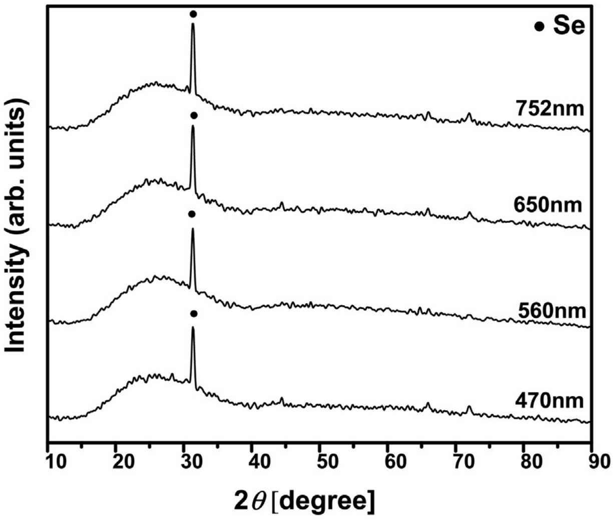

Fig. 1. X-ray diffraction patterns of $Se_{80}Te_8(NaCl)_{12}$ thin film of different thicknesses.

according to the best agreement between the observed of both diffraction angle and inter-planar spacing with those of Joint Committee on Powder Diffraction Standards (JCPDS). These standard are $2\theta = 31.51°$ and $d = 2.84$ Å. Accordingly, the crystallized phase in all deposited films is Se phase with a preferred orientation along the (101) direction having a hexagonal structure. The intensity increase of the (101) plane is explained by the improvement of the crystallinity of the film with increasing thickness.

3.2. Transmission and Reflection Spectra

The transmission spectrum of a clean glass substrate and that of the $Se_{80}Te_8(NaCl)_{12}$ thin films after subtracting the transmittance of the substrate are shown in Fig. 2. The transmittance of the substrate is around 90% in the range of 400–2500 nm, indicating a highly transparent material. For observed spectrum of any film, the transmission curve makes interference fringe patterns at various wavelengths in the infrared region. These interference patterns indicate a high structural perfection of the thin films [16]. The number of maxima and minima of the fringes, due to multiple reflections of the incident light are found to be increase as the thickness of the film is increased. The films show highly transparence reaching to about 90% in the visible and infrared regions. The transmittance for all film thickness increases as the wavelength of the incident photons increases until reach to a certain wavelength (λ) in the visible region. However, the transmittance threshold is slightly shifted to the longer wavelengths with increase of the film thickness indicating the reduction of the optical band gap as the thickness increases.

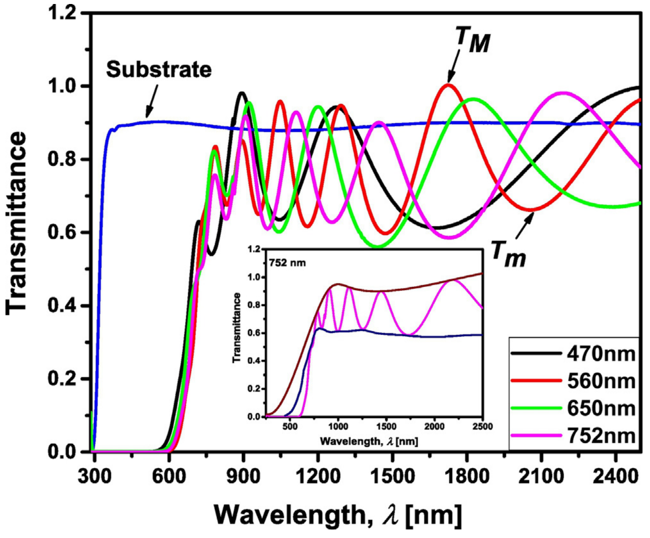

Fig. 2. Transmittance spectra of the substrate and $Se_{80}Te_8(NaCl)_{12}$ thin films as a function of the wavelength. The inset shows the constructing of the two envelopes for a transmission spectrum.

The reflection spectra of $Se_{80}Te_8(NaCl)_{12}$ film of the four different thicknesses are shown in Fig. 3. The reflectance shows successive up and down curvatures overall incident wavelength. The observed upward curvature in the transmittance together with the corresponding downward one in the reflectance at higher wavelengths is attributed to the interaction of light waves with the free carrier absorption [17].

3.3. Refractive Index and Thickness

The observed interference fringes in the transmittance spectrum motivate to use them to gain information about the dispersion and thickness of the investigated film materials using Swanepoel method. This method is applicable in the case of a weakly absorbing thin film on an entirely transparent substrate that is much thicker than the thin film. In addition as shown from the inset of Fig. 2, the created upper and lower envelopes of the transmittance spectrum are almost parallels to the *x*-axis indicating the homogeneity of the film material. It is worth noting that these conditions are met in this work [18]. Constructing the two envelopes for the experimental transmission spectrum of a film/substrate sample and knowing transmission of the clean substrate alone make possible the determination of the refractive index and thickness of the film.

The refractive index (n) of the film in the region where absorption coefficient (α) ≈ 0 can be calculated using the equation [19]

$$n = \left[N + \left(N^2 - s^2\right)^{\frac{1}{2}}\right]^{\frac{1}{2}} \tag{1}$$

where s is the refractive index of the glass substrate and N is given by

$$N = \frac{1}{2}\left(s^2 + 1\right) + 2s\frac{T_M - T_m}{T_M T_m}, \tag{2}$$

where T_M and T_m are the maximum and minimum transmittances at the same wavelength in the envelope curve on the transmittance spectrum.

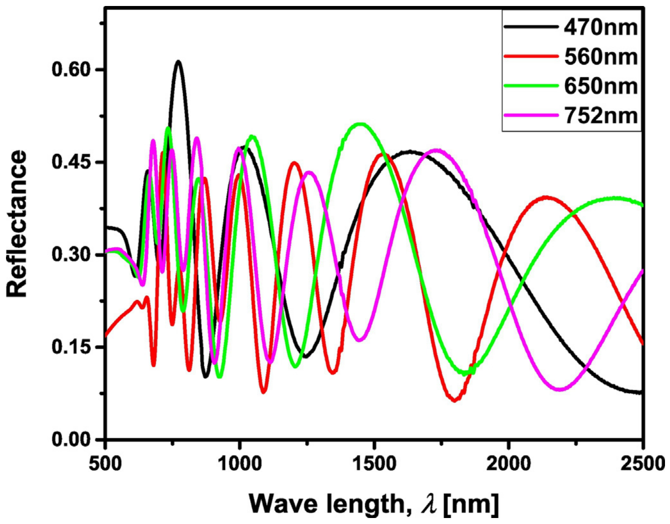

Fig. 3. Reflectance spectra of $Se_{80}Te_8(NaCl)_{12}$ thin films as a function of the wavelength.