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Optical properties of a-As₂Se₃ thin films

Abstract. Chalcogenide glassy semiconductors currently have found widely applications in the opto- and microelectronics devices. On this work we studied the optical properties of amorphous a-As₂Se₃ thin films which were produced on the quartz substrate by thermal evaporation method with different thickness: 500 nm, 1000 nm, 2000 nm. The transmission spectra were measured by spectrophotometer in the spectral range 250 -1000 nm. It is known that Swanepoel method can be used to determine the frequency dependent refractive index of thin films via interference fringes of transmission spectra. Using the obtained transmission spectrum and Swanepoel's method we calculated the optical constants of a-As₂Se₃ thin films in the 700 – 900 nm wavelength range. The found optical constants of a-As₂Se₃ films were used to theoretically determine the transmission spectrum by the matrix transfer method (TMM). The comparison of theoretical and experimental values of transmittance was made and proved the practical usage of these methods.

Key words: a-As₂Se₃ thin films, transmission spectrum, refractive index, Swanepoel's method, transfer matrix method.

Introduction

During the last several years the interest in chalcogenide glassy semiconductors grew remarkably. Chalcogenide glasses thin films are produced by various methods such as thermal evaporation, sputtering, chemical vapor deposition etc [1]. Many attractive materials have been selected up to now. One of them is As₂Se₃ which was prepared by direct fusion of high-purity As and Se and has excellent infrared transmission characteristics [2]. They are useful material for optical elements [3], optical memory disks [4], functional elements in integral-optic systems [5], IR-fibres [6] that show high flexibility and chemical durability [7] etc.

Chalcogenide glasses based on Se have good thermal, mechanical and chemical properties and they are used as materials for electronic and optoelectronic devices [8]. The fundamental issue of amorphous semiconductors is to analyze the difference in characteristics between the crystalline and the amorphous phase [9].

The optical properties of the material depend on the optical band gap, refractive index and extinction coefficient. It is quite essential to know the material's atomic structure, electronic band structure and electrical properties [10]. We can easily calculate the optical constants of materials using transmittance and reflectance spectra. During the experimental work, we determined the optical properties of As₂Se₃ by using a variety of thin films of different thickness.

Experiment

As₂Se₃ thin films were produced by thermal evaporation method in VUP-5 equipment. The spectra of optical transmittance and reflectance of the obtained thin films were measured using Shimadzu UV-Vis spectrophotometer. The transmittance and reflectance spectra of As₂Se₃ thin films with different thickness 500 nm, 1000 nm and 2000 nm are represented on Fig. 1. The thickness of films was determined by Scanning Electron Microscope, Quanta 3D 200i.

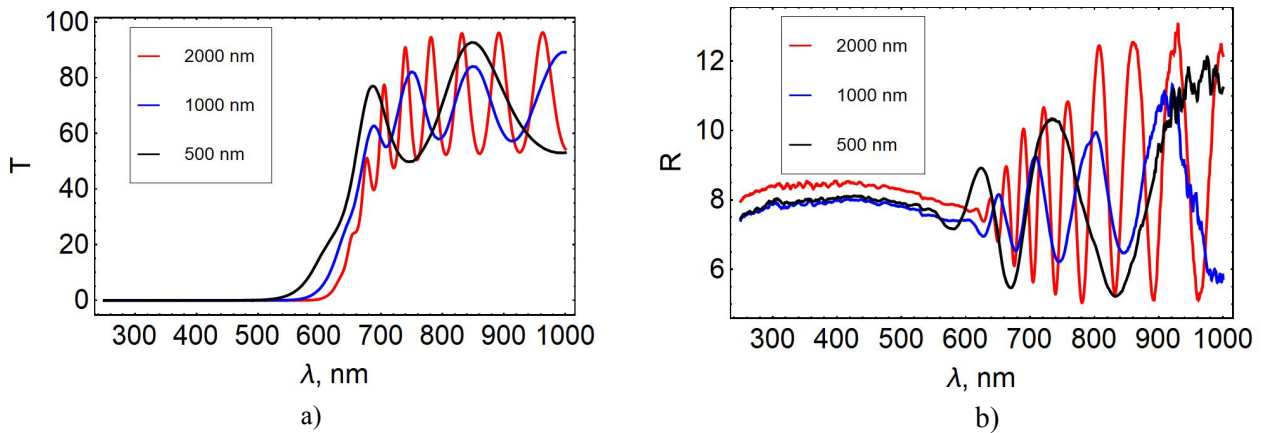


Figure 1 – The transmission (a) and reflection (b) spectra of a-As₂Se₃ films obtained by thermal evaporation

Swanepoel’s method for determination of optical constants

The optical transmission measurement of film-on-substrate system which is shown in Fig. 2 has semitransparent or transparent films and the finite thickness of the substrate d_s which is several orders of magnitude larger than the film thickness d [11].

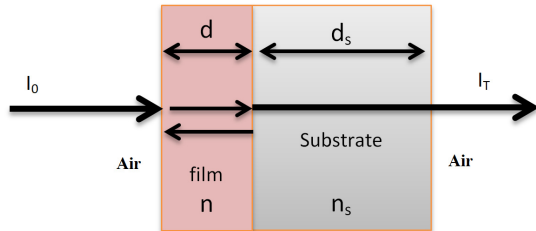


Figure 2 – Schematic illustration of light transmission through a film-substrate system

The total transmission $T(\lambda)$ by Swanepoel’s method:

$$T(\lambda) = \frac{Ax}{B - Cx \cos \varphi + Dx^2} \tag{1}$$

Optical constants of thin films described with complex refractive index $n_c = n + ik$, n – the refractive index, k - the extinction coefficient which can be found as

$$k = \alpha\lambda/4\pi, \tag{2}$$

where α denotes absorption coefficient of As₂Se₃ films.

The absorption coefficient α can be calculated in the strong absorption region by taking into account measured values of R and T:

$$\alpha = \frac{1}{d} \ln \left(\frac{(1-R)^2 + [(1-R)^4 + 4R^2T^2]^{\frac{1}{2}}}{2T} \right) \tag{3}$$

The refractive index $n(\lambda)$ can be found using Swanepoel’s method:

$$n = [N + (N^2 - s^2)^{1/2}]^{1/2}, \tag{4}$$

where

$$N = 2s \frac{T_M - T_m}{T_M T_m} + \frac{s^2 + 1}{2} \tag{5}$$

Those equations are enough to calculate optical constants of the thin films. The T_m and T_M were obtained by transmittance spectra and presented with puncture lines on Fig. 3, s – is a refractive index of quartz substrate, $s=1.55$. The Fig.4 shows the refractive index and extinction coefficient of As₂Se₃ which are found using (2) and (4) for thickness of 2000 nm.

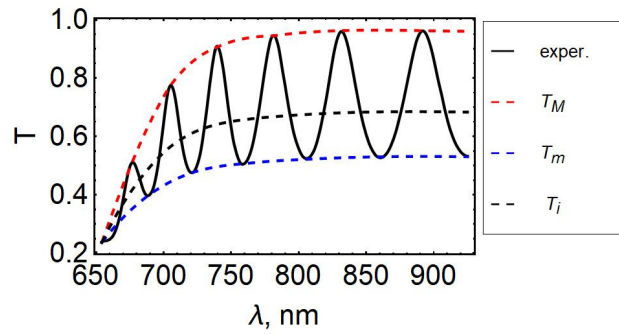


Figure 3 – The reflection spectrum of a-As₂Se₃ films obtained by thermal evaporation

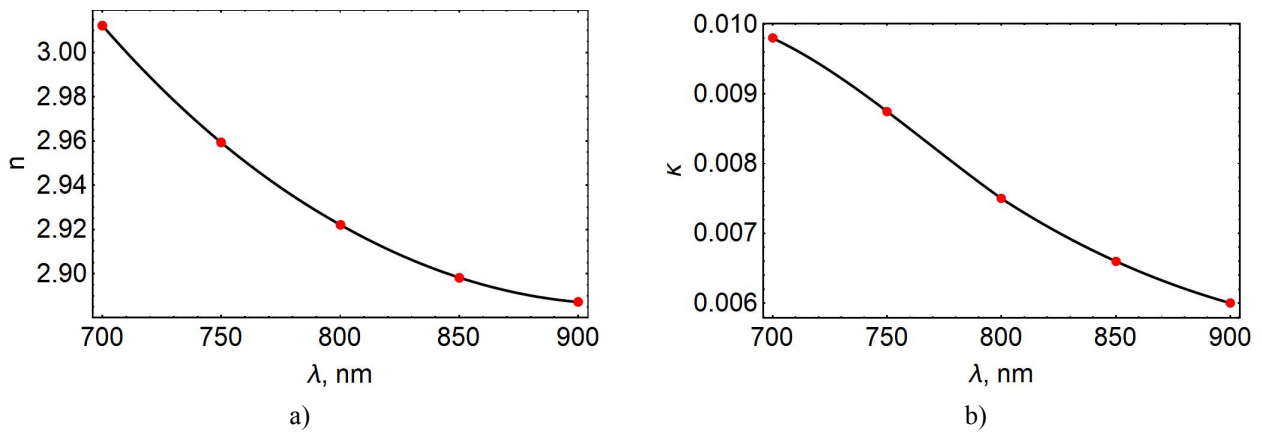


Figure 4 – The refractive index (a) and extinction coefficient (b) of a-As₂Se₃ films determined according to the Swanepoel’s method

Transfer Matrix Method

Using Transfer Matrix Method and values of refractive coefficient it is possible to calculate transmittance on layered structures. The basic formula for wave propagation on layered systems has the following form:

$$\begin{bmatrix} E_1^+ \\ E_1^- \end{bmatrix} = T \begin{bmatrix} E_{N-1}^+ \\ E_{N-1}^- \end{bmatrix}, \tag{6}$$

where E_1^-, E_1^+ – backward and forward amplitudes of incidence wave, E_{N-1}^+ – transmitted wave amplitude and T is the transfer matrix which is obtained by multiplying: the transition matrix $T_{i \rightarrow j}$ through the interface, and the propagation matrix in a dielectric medium $P_i(d)$. In our case, T is determined as

$$T = T_{0 \rightarrow 1} P_1(d) T_{1 \rightarrow 2}. \tag{7}$$

The transition matrix $T_{i \rightarrow j}$ defined as follows:

$$T_{i \rightarrow j} = \frac{1}{t_{i,j}} \begin{bmatrix} 1 & r_{i,j} \\ r_{i,j} & 1 \end{bmatrix}. \tag{8}$$

For TE-polarization:

$$r_{ij} = \frac{n_j \cos \theta_i - n_i \cos \theta_j}{n_j \cos \theta_i + n_i \cos \theta_j}, \tag{9}$$

$$t_{ij} = 1 + r_{ij} = \frac{2n_i \cos \theta_i}{n_j \cos \theta_j + n_i \cos \theta_j}, \tag{10}$$

and for TM-polarization:

$$r_{ij} = \frac{n_j \cos \theta_i - n_i \cos \theta_j}{n_j \cos \theta_i + n_i \cos \theta_j}, \tag{11}$$

$$t_{ij} = \frac{n_i}{n_j} (1 + r_{ij}) = \frac{2n_i \cos \theta_i}{n_j \cos \theta_j + n_i \cos \theta_j}. \tag{12}$$

Propagation matrix in As_2Se_3 layer is written by following form

$$P_i = \begin{bmatrix} e^{-k_{x,i}d_i} & 0 \\ 0 & e^{k_{x,i}d_i} \end{bmatrix}. \quad (13)$$

The transmission coefficient Tr at normal incidence of wave can be obtained by using simple relation:

$$Tr = \left| \frac{1}{T_{11}} \right|^2. \quad (14)$$

Figure 5 represents the comparison of transmission coefficient of 1000 nm thick As_2Se_3 film determined by numerical results based on TMM with experimental measurements. The small difference in the spectra in Fig. 5 is probably due to the inhomogeneity of the film thickness in which interference is observed.

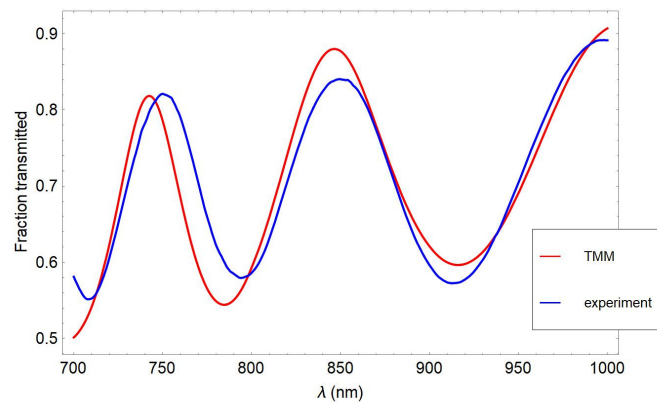


Figure 5 – Comparison of theoretical and experimental results of transmission spectrum of As_2Se_3 thin films

Conclusion

Thin As_2Se_3 films were produced by thermal evaporation method with different thickness 500nm, 1000nm, 2000nm. Swanepoel's method is used to evaluate the values of refractive index and extinction coefficient which are in a good agreement with the results of other authors. The refractive index and extinction coefficient were found in the range of 700 nm - 900 nm. The found coefficients were used to theoretically determine the transmission spectrum by the matrix transfer method. The theoretical and experimental results have some slight difference due to non-uniform thickness of thin films. According to the result, it can be concluded that the transfer matrix method gives adequate results and can be used to predict the optical characteristics of thin films and their layered structures.

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