The Dispersion Energies Wemple-Didomenico in Nanomultilayers Based on As_2S_3-Se and $Ge_5As_{37}S_{58}$-Se Chalcogenide Glasses

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***Abstract* — The dispersion energies and the single oscillator energies were calculated using the optical transmission data in amorphous chalcogenide nanomultilayers based on As_2S_3–Se and $Ge_5As_{37}S_{58}$–Se. It is shown that the dispersion parameters of these structures can described by the Wemple–DiDomenico refractive–index model.**

***Key words* — Amorphous chalcogenide, nanomultilayers, single oscillator model.**

I. INTRODUCTION

S. H. Wemple and M. DiDomenico [1] have analyzed the refractive-index dispersion data below the interband absorption edge in covalent and ionic materials. They have shown that spectral dependence of refractive index can be well described by single effective oscillator model. According to this model refractive index is related to energy of incident photon by equation $n^2 - 1 = E_d E_0 /(E_0{}^2 - E^2)$ that can be used in a wide range of different solids and liquids. Here the E is the photon energy, E_0 is the single oscillator energy that determines the position of effective oscillator connected with average energy gap, and E_d is the dispersion energy. The latter energy is a measure of the strength of interband optical transitions. It was also found [2] that the mentioned relationships can be applied to a variety of optical glasses and amorphous semiconductors, mainly in tetrahedral materials and mixed –oxide glasses. An example was given also for amorphous As_2S_3, Se and Te monolayers. In [3] it was found that even in the case of ternary amorphous films with complex short and medium range order the dispersion parameters can be described by the Wemple-DiDomenico refractive-index model.

In present investigation the dispersion energies E_d and E_0 and also optical band gap energy E_g are calculated both for As_2S_3-Se, $Ge_5As_{37}S_{58}$-Se multilayer nanostructures and As_2S_3, $Ge_5As_{37}S_{58}$ and Se layers.

II. MATERIALS AND METHODS

Amorphous As_2S_3-Se and $Ge_5As_{37}S_{58}$–Se nanomultilayers structures were prepared by computer driven cyclic thermal vacuum deposition from two isolated boats with As_2S_3 or $Ge_5As_{37}S_{58}$ and Se on constantly rotated substrate at room temperature in one vacuum deposition cycle. The control of the thickness was carried out in-situ during the thermal evaporation by interference thickness sensor at λ=0.95µm. Overlapping part of samples contained alternating nanolayers of As_2S_3 or $Ge_5As_{37}S_{58}$ and Se, and control layers of As_2S_3 or $Ge_5As_{37}S_{58}$ and Se were deposited at the same time onto the same substrate consequently through masks and used to check the composition and calculate the ratio of the sub-layer thicknesses in one modulation period. Thicknesses of constituent sub-layers of nanomultilayer structure are sufficiently smaller than light wavelength. So it was possible to use in the analysis of optical transmission spectra of nanomultilayers the "effective optical medium" model: the layers, with smaller E_g value, determine the optical absorption at the average absorption edge E_g, and the "barrier" layers with larger E_g are transparent.

The dispersion energies were determined from the experimental results on the optical transmission measurements with refractive index dispersion calculation. Spectrophotometer Specord M40 was used for the transmission measurements covering the spectral range of 200-900 nm. Swanepoel method [4] was used to calculate the dispersion of refractive index n, absorption coefficient α and the thickness d of investigate samples. The determination of the optical bandgap energy E_g was done by extrapolating Tauc's plot [5] for indirect bandgap material: $(\alpha h\nu)^{1/2}=f(h\nu)$.

III. RESULTS AND DISCUSSION

Figure 1 shows the refractive index (n) dispersion curves of As_2S_3-Se and $Ge_5As_{37}S_{58}$-Se multilayer nanostructures and As_2S_3, $Ge_5As_{37}S_{58}$ and Se pure layers, which were calculated from the transmittance spectra of thin films. Once the refractive index dispersion was obtained, the value of static refractive index n(0) was obtained by extrapolating Wemple-DiDomenico relation in low energy limit (hν→0) and energies E_d and E_0 were calculated by means of the plot of $(n^2-1)^{-1}$ versus E^2 [1]. This relation is valid only for photon energies less than optical bandgap. Linear least square fitting of $(n^2–1)^{-1}$ with $(E)^2$ was obtained using OriginPro 8.1 (Originlab).

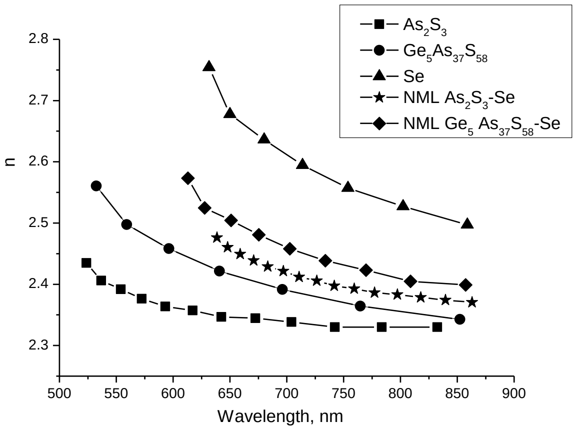

Fig. 1. Refractive index dispersion of As$_2$S$_3$-Se and Ge$_5$As$_{37}$S$_{58}$-Se nanomultilayers and As$_2$S$_3$, Ge$_5$As$_{37}$S$_{58}$ and Se pure layers.

For the nanomultilayers structures Ge$_5$As$_{37}$S$_{58}$ and As$_2$S$_3$ and Se layers the spectral dependencies of refractive index factor $(n^2 – 1)^{-1}$ versus the photon energy squared E^2 are shown in Fig.2.

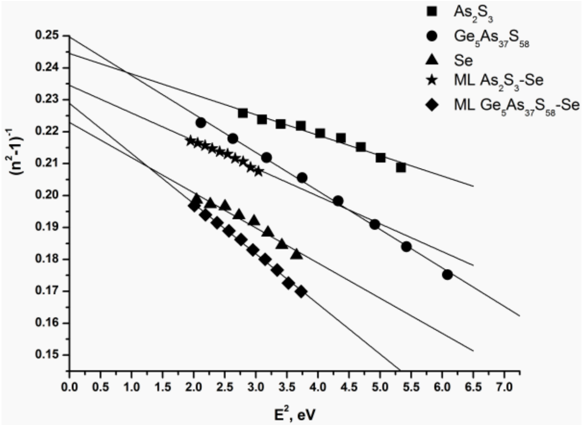

Fig. 2. Plot of the refractive index factor $(n^2 – 1)^{-1}$ versus the photon energy squared E^2 to determine values of E_d and E_0.

Optical parameters evaluated from transmission spectra together with thickness *d* are given in the Table I. It can be seen from the data given in this table that E_0 scales well with the optical band gap ($E_0 \approx 2 \times E_g$), which is in accordance with the results reported in [6,7].

TABLE I. OPTICAL PARAMETERS OBTAINED FROM TRANSMISSION SPECTRA

Structure composition	d, nm	n(0)	E_d, eV	E_0, eV	E_g, eV
Se layer	1590	2.342	20.345	4.537	1.92
As$_2$S$_3$ layer	1500	2.243	23.767	5.895	2.34
As$_2$S$_3$-Se nanomultilayers	3090	2.292	21.911	5.149	1.94
Se layer	1030	2.32	15.4	3.52	1.92
Ge$_5$As$_{37}$S$_{58}$ layer	730	2.25	18.9	4.63	2.3
Ge$_5$As$_{37}$S$_{58}$-Se nanomultilayers	1760	2.33	16.9	3.83	1.92

IV. CONCLUSIONS

Thin film structures of As$_2$S$_3$-Se and Ge$_5$As$_{37}$S$_{58}$-Se nanomultilayers and As$_2$S$_3$, Ge$_5$As$_{37}$S$_{58}$ and Se pure layers were prepared and analyzed for their refractive index dispersion by means of transmittance spectra over the wavelength range: 400 – 900 nm.

The single oscillator energy, E_0, dispersion energy, E_d, and optical band gap, E_g were calculated from the data of optical transmission measurements in As$_2$S$_3$–Se and Ge$_5$As$_{37}$S$_{58}$–Se chalcogenide nanomultilayers. Spectral dependences of refractive index *n* obtained by Swanepoel method were studied. It was found that even in the case of nanomultilayers structures with complex short and medium range order the dispersion parameters can be described by the Wemple–DiDomenico refractive index model (single oscillator model).

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