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Structural and optical properties of evaporated Ge/Al Bilayer thin films

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Abstract

Germanium- aluminum (a-Ge/Al) bilayer thin films with two different Al thicknesses were deposited onto glass substrates by thermal evaporation technique. The structural and optical properties were investigated and the effect of Al layer thickness on film properties was discussed. X-ray diffraction (XRD) confirmed the amorphous nature of the films under study. The small values of the roughness (7.04 nm, 7.2 nm) obtained from atomic force microscopy (AFM) measurements show relatively smooth surfaces. The optical properties of aGe-Al bilayer thin films were determined from the analysis of measured spectroscopic ellipsometry over the wavelength range 300-1000 nm at room temperature. The refractive index, extinction coefficient and thicknesses were obtained by the analysis of the ellipsometric spectra through Cauchy, and the Tauc-Lorenz models. have been calculated. The optical energy gap was estimated from the absorption coefficient values which were estimated from the absorption coefficient values using Tauc's procedure. Our results show that the optical band gap decreases with increasing Al layer thickness.

Keywords: Optical properties, Spectroscopic ellipsometry, Ge/Al bilayer thin films
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1. Introduction

Thin amorphous germanium (a-Ge) films are very interesting due to their wide utilization in different applications, such as diode technology, photovoltaic cells, and photorefractive devices [1-4]. Recently, it was found that the crystallization process of amorphous semiconductor layers is occurring when depositing these layers on certain metals. Crystallization of a-Ge layer occurs at the original a-Ge/Al interface [5-8]. Wang *et*

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[12], we found an intense diffraction at 26.189°, which may be assigned to the Ge (111) plane, along with two weak broadened diffraction peaks at 44.740° and 45.306°, that may assigned to the diffraction of Al (200) and Ge (220) planes, respectively. Fig. 1, also shows a relatively intense broadened diffraction peaks, one at 2θ = 27.284° which corresponds to the diffraction from Ge (111), while there are two sharp clear peaks at 2θ = 29.655° correspond to the diffraction from Ge (102) plane, and 2θ = 33.395° corresponds to the diffraction from Ge (112). The third sharp peak at 2θ = 38.473° results from the Al (111) plane. The appearance of these peaks clearly shows an increase in intensity, which might be attributed to improvement of crystallinity with increasing Al layer thickness.

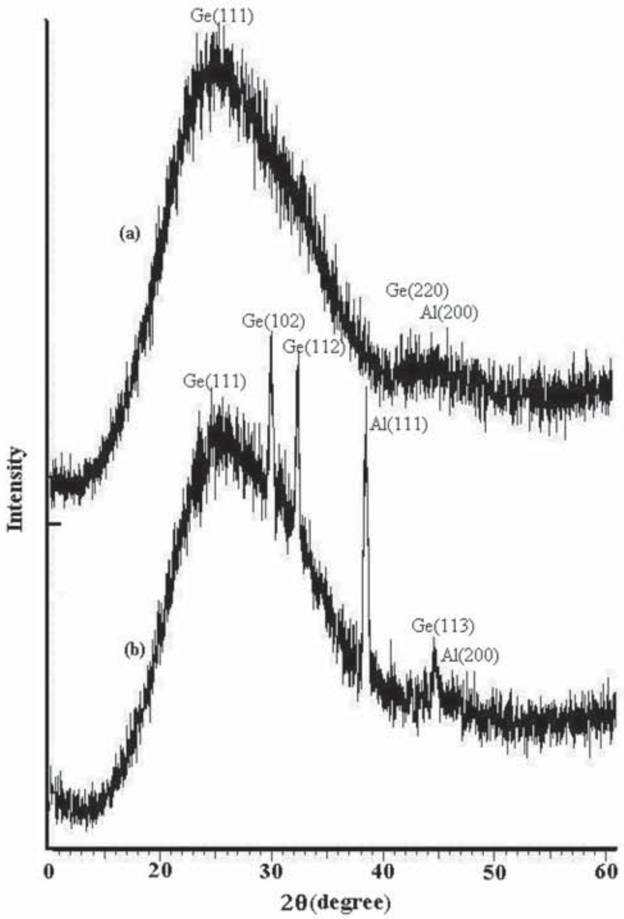

Fig. 1: X- ray diffraction spectra of amorphous Ge-Al bilayer thin films for (a) 10 nm Al layer and (b) 50 nm Al layer

The surface morphology of Ge/Al thin films has been investigated by AFM. Fig. 2 (a) and (b), shows the AFM images (2 μm × 2μm) of these thin films. It is shown that the films are adherent on glass substrates, smooth, and pinhole free. The values of root mean square (rms) surface roughness were 7.2 nm, and 7.04 nm for samples 1 and 2, respectively. These results indicate that the surface quality of Ge/Al films is smooth, which is considered as an important property for the coatings that are used for interferometric applications in order to reduce the reflection loss due to roughness induced surface scattering.

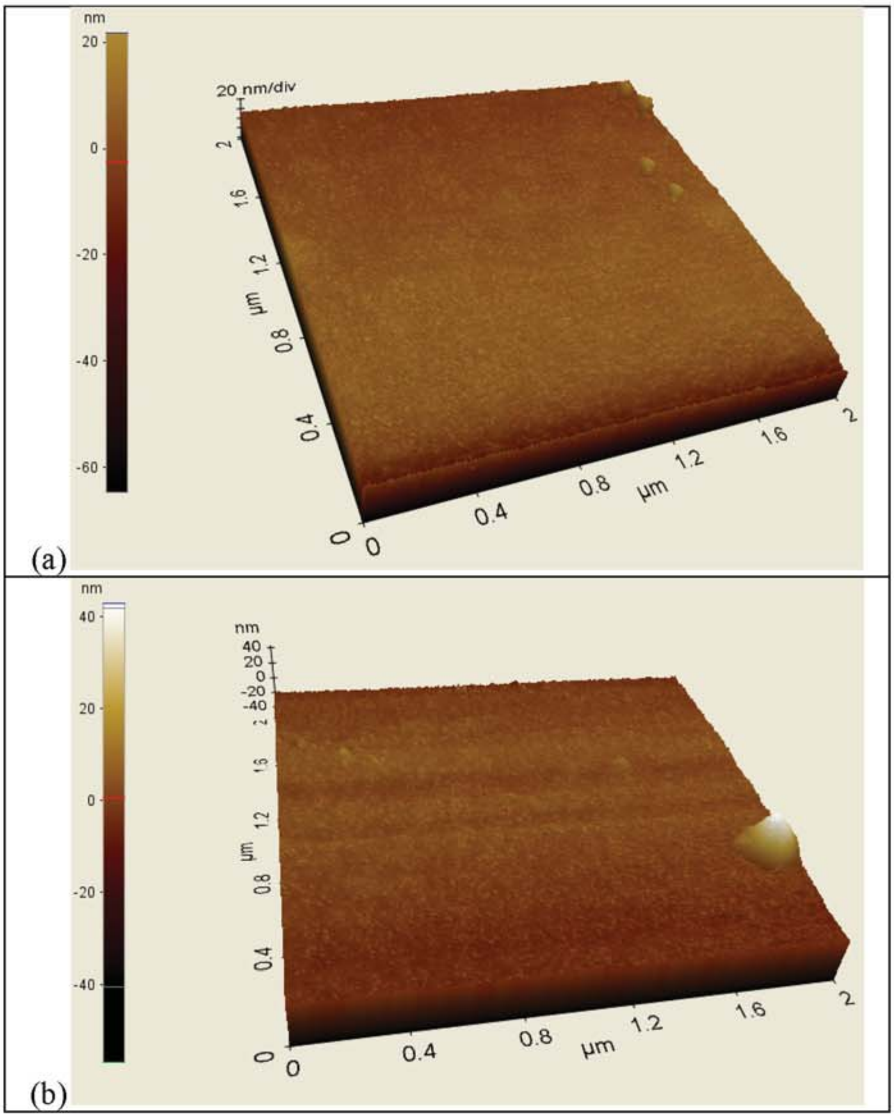

Fig. 2: AFM images (2×2 μm area) of Ge-Al bilayer thin films for (a) 10 nm Al layer and (b) 50 nm Al layer

The dispersion model for transparent materials such as bulk glass is best modeled by Cauchy dispersion relation that describes the index of refraction (n) as a function of incident light wavelength (λ) by

$$n(\lambda) = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4} \tag{1}$$

where the Cauchy constants being A=1.4987 , B=0.00462 nm^2 , and C=-0.00016 nm^4, are the fitting parameters for the used glass substrate. The parameter values agree well with the reported values [13]. Extinction coefficient (k) vanishes in the visible region (400-700 nm). The fitting parameters and the number of backside reflections from the backside surface of the glass substrate were set to vary in order to fit for the Ψ data only. The 90% confidence factor, the fitting parameters in the fitting parameters correlation matrix and the minimum biased test function mean square error (MSE), as defined by Levenberg- Marquadrat algorithm, were all used as indicators of good confidence for the regression analysis and the data fitting.

Fig. 3 shows the model and recorded spectra taken for two samples 1 and 2. The model spectra were generated using Tauc-Lorentz (TL) model [14] using five TL parameters to represent Ge layer. A best fit was achieved according to [glass/ Ge/ Al/ Al_2O_3] model shown in Fig.3(a). The measured spectroscopic ellipsometry data, Ψ and Δ, of a-G/Al thin films at two angles of incidence, namely, 70° and 75° are given in Figs. 3(b,c).The fitted Ψ and Δ spectra, simulated with the best-fit TL model parameters, are presented by solid lines. The fitting was performed by minimizing the mean square error (MSE) [15], with layer thicknesses, and five TL parameters. A good fitting with MSE values of 7.264 and 3.065 were obtained for the desired wavelength range. Table 1 contains the values of layer thicknesses, and TL parameters for the two samples. The values of the same parameter for these two samples are close, which indicates the validity of the used model.

Al_2O_3
Aluminum
Germanium (Tauc-Lorenz)
Bulk glass substrate

Fig. 3(a)

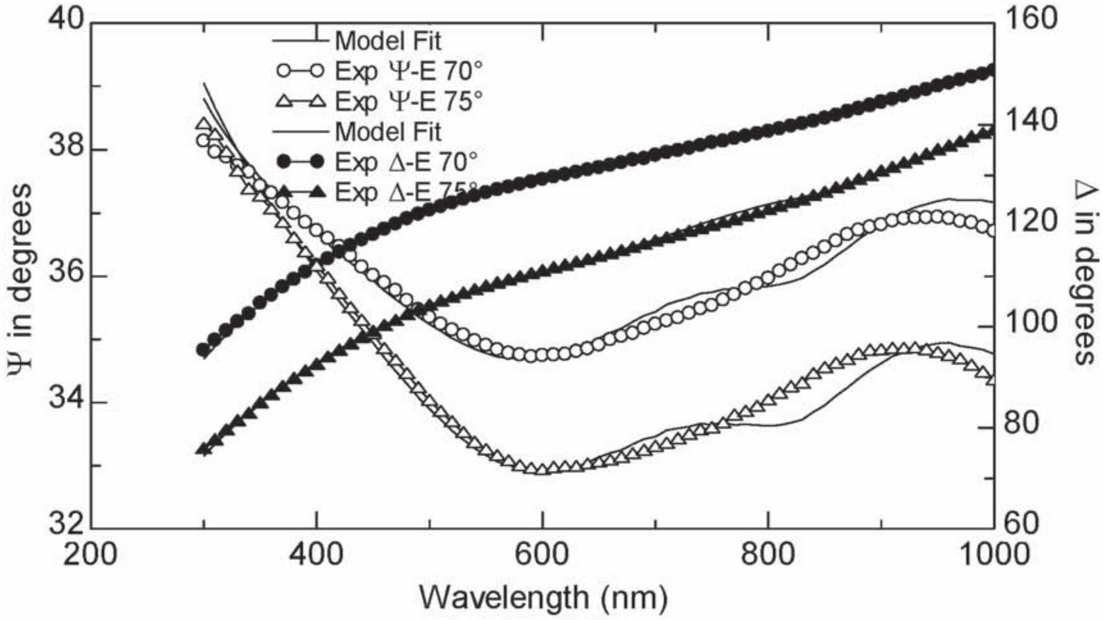

Fig. 3(b)

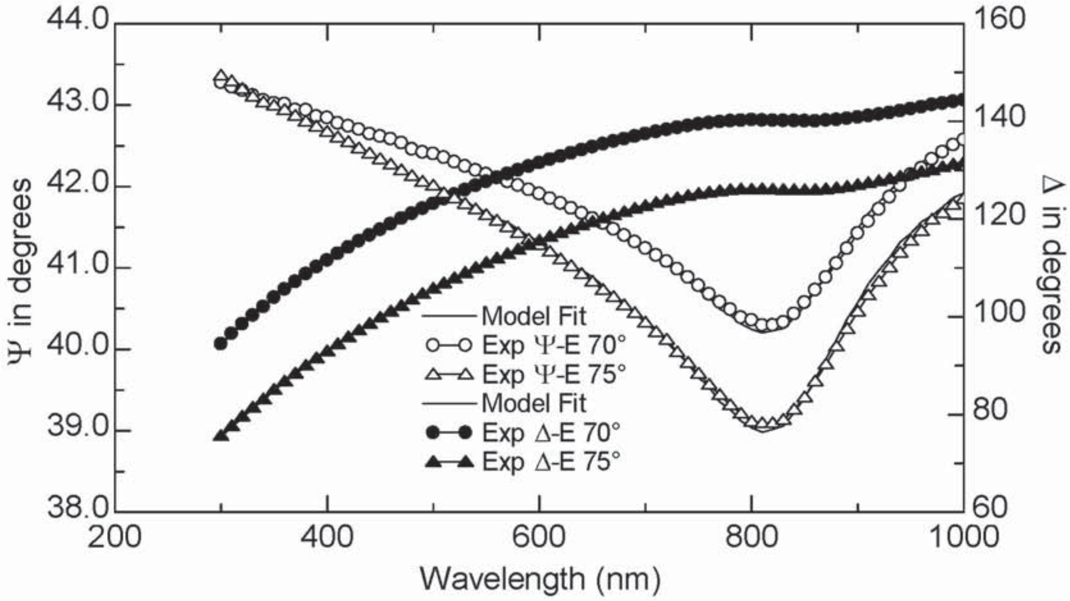

Fig. 3(c)

Fig. 3: (a) The model used in the fitting procedure (b) The measured ellipsometric Ψ and Δ together with the best fitting (solid line) for sample 1. (c) The measured ellipsometric Ψ and Δ together with the best fitting (solid line) for sample 2.

Table 1: The resulting fitted thicknesses and parameters of the Tauc-Lorentz model for samples 1 and 2. The 90% confidence limits are given by (±).

Sample	a-Ge Thickness (nm)	Tauc-Lorenz Parameters E_i (eV)	A $(eV)^2$	E (eV)	C (eV)	E_g (eV)	Al Thickness (nm)	Al_2O_3 Thickness (nm)
1	50.269±4.60	1.1278	35.465	6.053	8.568	0.7662	10.026±1.06	3.632±0.09
2	50.898±6.19	2.6228	37.146	7.379	8.568	1.3293	52.656±1.85	1.667±0.01

The refractive index and extinction coefficient of samples 1 and 2 are shown in Figures 4 and 5. Refractive indices (Fig. 4) were found to be in the range (4-4.85), while the extinction coefficients (Fig. 5) were in the range (0-3). It is clearly apparent from Fig. 4 that *n* is increasing with increasing the photon energy, then decreasing showing a broadened peak value. It is shown also that the peak position of sample 2 is shifted towards higher photon energy.

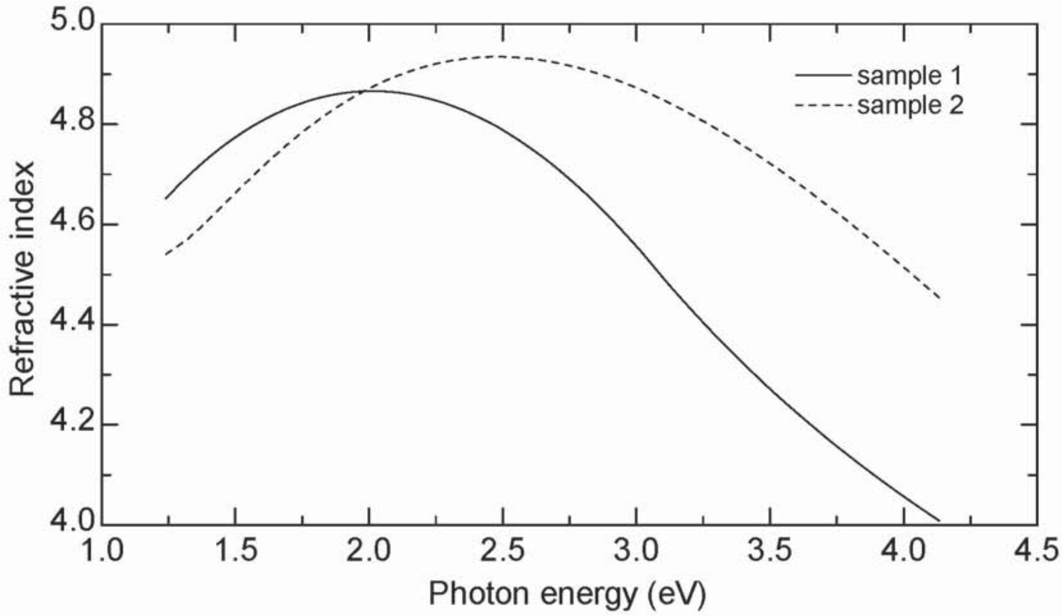

Fig. 4: Refractive index for Ge layer for samples 1 and 2 as a function of photon energy.

Fig.5 shows an increasing in the extinction coefficient (k) values with increasing photon energy.

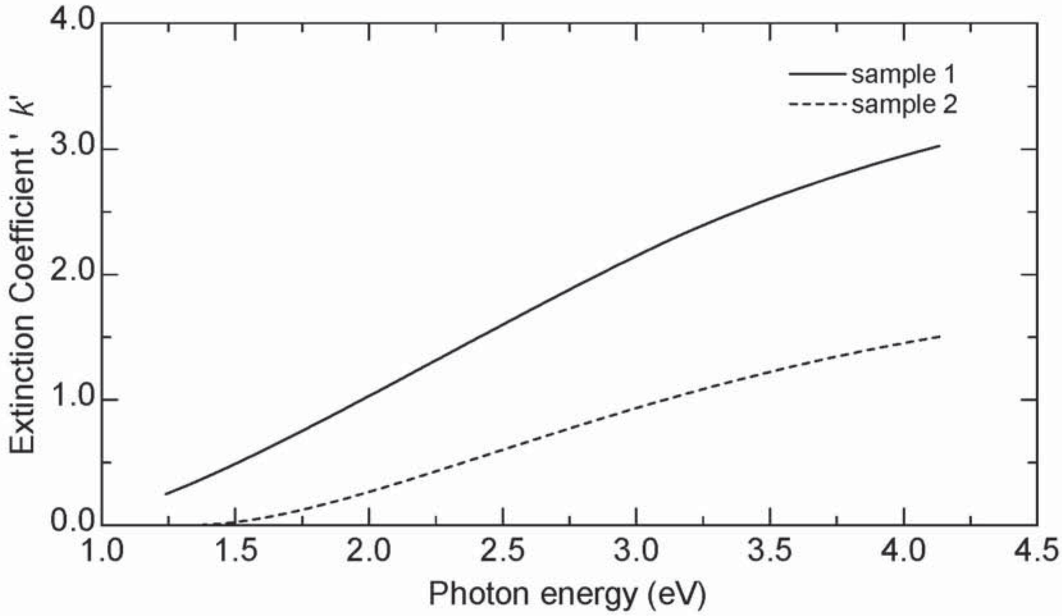

Fig. 5: Extinction coefficient for Ge layer for samples 1 and 2 as a function of photon energy.

The above ellipsometric studies were considered as productive tools for understanding the optical band gap of Ge/Al bilayer thin films. The study of the absorption coefficient spectrum (α) of a semiconductor in the fundamental region and near the fundamental edge provided us with valuable information about the energy and structure of the material. It is well known that the shape of the fundamental absorption edge in the exponential region can yield information on the disorder effects [16]. The lack of crystalline long range order in amorphous materials is associated with a tailing of density of states [17]. The values of absorption coefficient (α) as a function of photon energy (*hυ*) were obtained in Fig. 6.

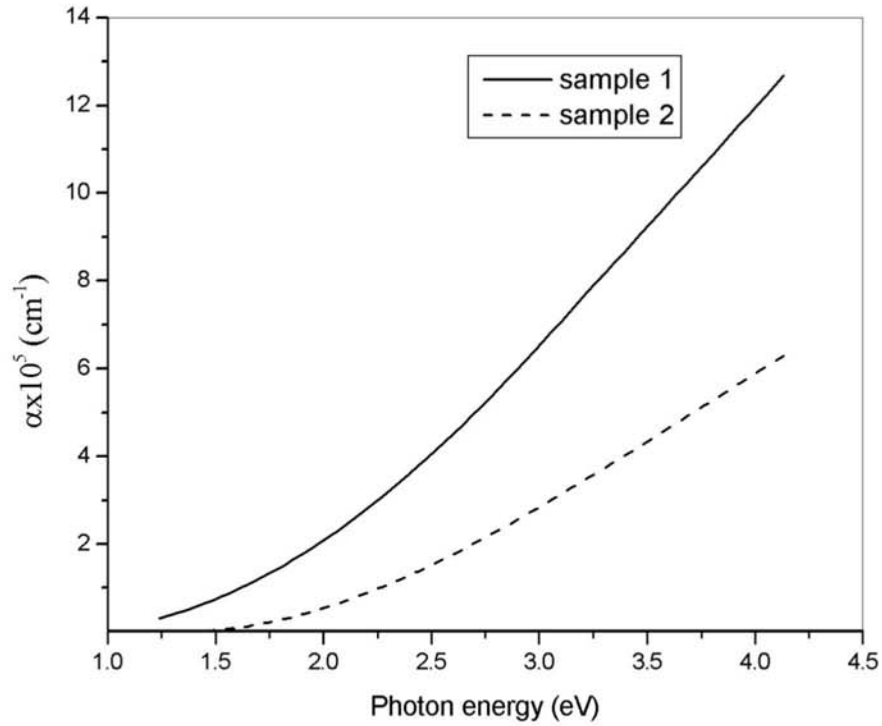

Fig. 6: Absorption coefficients of a-Ge layers in samples 1 and 2 as a function of photon energy.

It is obvious that α values are of the order 10^5 cm^{-1}, leading to the conclusion that the films are of the indirect band gap type and the transitions are allowed. It is clear from Figure 6, that α increases from 0.05×10^5 to 1.2×10^6 cm^{-1} with increasing photon energy in the region of 1.25-4 eV. Below 2 eV, α exhibits a tail in the absorption curve. The existence of this tail may be attributed to the amorphous nature of Ge and/or randomly distributed impurities in the films [18]. On the other hand, there are two distinct regions this figure, the first is the exponential edge region, which is strongly related to the structural randomness of the system, and the second is the high absorption region that determines the optical energy gap.

The absorption coefficient α of the investigated Ge/Al bilayer thin films can be calculated using Tauc equation as follows [19]:

$$\alpha(\nu) = \beta(h\nu - E_g)^2 / h\nu \qquad (2)$$

where E_g is the electronic energy gap and β is an energy independent constant. According to equation (2), the $(\alpha h\nu)^{1/2} = f(h\nu)$ dependencies are linear, which characterizes indirect electron transitions between the maximum of valence band and the minimum of conduction band. E_g can be determined by extrapolating these linear portions to $(\alpha h\nu)^{1/2} = 0$. The corresponding energy gap determined from Fig.7 at about 0.908 eV for sample 1, and 1.402 eV for sample 2.

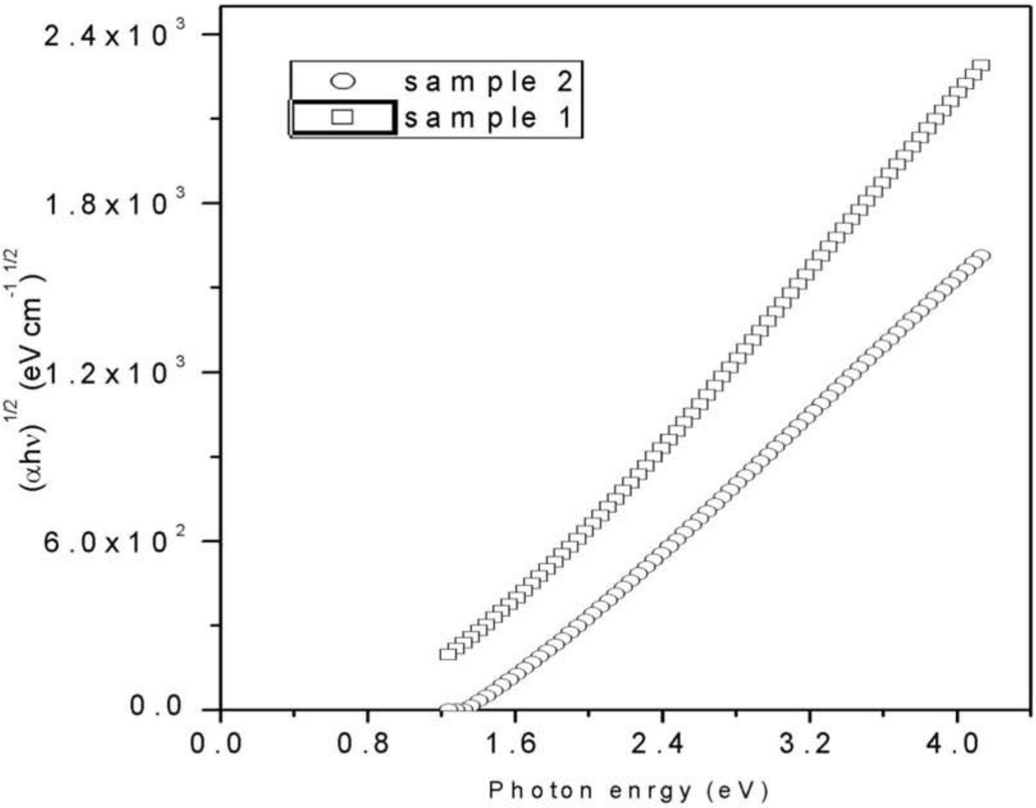

Fig. 7: Plots of $(\alpha h\upsilon)^{1/2}$ as a function of photon energy of Ge layer for samples 1 and 2.

This change might be attributed to the increase in Al-Ge bonds. Al enters into the structure of Ge forming units containing both elements, leading to a modified network. Further, the optical band gap is strongly dependent on the fractional concentration of atoms.

4. Conclusions

Germanium aluminum bilayer thin films were successfully prepared by evaporation on glass substrates. The X-ray data indicate that the germanium covered by thinner Al layer is of amorphous nature, while the appearance of diffraction peaks in a second sample with thicker Al layer indicates to improvement of material crystallinity. From AFM images, the root mean square roughness was found to have a relatively small values, which indicates the smoothness of film surfaces. The ellipsometric spectra of the films were recorded in the incident wavelength range of 300-1000 nm. The Tauc-Lorentz model was applied for the germanium layer to determine the refractive index, extinction coefficient and wavelength dependence. The absorption coefficient was also calculated and show short band tails at low absorption coefficient values ($\alpha \sim 10^4$ cm^{-1}). Moreover, the structure, morphology and optical properties of the film depend on Al layer thickness, which is important for several metal-semiconductor applications.

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