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The effect of Bi content on the optical energy gap width of the amorphous thin films system $Se_{85}Ge_{15-x}Bi_x$

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ABSTRACT

Thin amorphous films of Se85Ge15-$_x$Bi$_x$system, where(x = 0, 5, 10, 15, at %) were prepared by alloying the spec. pure raw materials using the common melt quenching technique. Using the thermal evaporation technique to form the required films. The films where checked by XRD and EDX to ensure the amorphous structure and composition of each sample. The optical properties (Transmittance T, Reflectance R) and the optical constants (Refractive index n, Extinction coefficient k, Absorption coefficient , were studied at the wave length range from 400 – 2500 nm. The optical energy gapof the films was calculated for thissystem.Usingthe absorption coefficient values for each Bi concentration which showed that the energy gap decreased on increasing the Bi content in the sample from 1.8eV to 1.2eV, which is attributed to the increase of the localized states leading to the reduction of the optical energy gap in the samples.

INTRODUCTION

Chalcogenide materials are subject to systematic research work due to the change of their physical and chemical properties in a wide range of environmental parameters[(1, 2)] . Thin films of Chalcogenide materials could be used as wide band gap high power devices, and high sensitive infrared detectors. They behave as semiconductors with band gap energy ranging from 1 eV to 3 eV[(3-5)]. Thin film materials with high optical transparency, could be used as flat panel displays, light sensors, optical limiters, and a variety of other devices that depend on the nonlinear optical response of their components[(6-8)].
The studies of the optical constant of such materials showed that these materials could be useful if were used in the manufacturing of optical fibers and reflecting coating. This can be related to their atomic structure as well as their electronic band structure[(9-11)].
The amorphous chalcognides, in particular, Germanium containing chalcogenides have many applications. The Bismuth addition induced structure modifications in the Germanium-selenium matrix. This is very clear in the studying of Bismuth effect of the optical energy gap[(12, 13)].
The aim of the present work, is to study the effect of Bismuth addition to the Ge-Se parent alloy on the optical energy band gap of the system $Se_{85}Ge_{15-x}$, where, x = 0, 5, 10, 15 at%.

MATERIALS AND METHODS

Sample preparation:
Preparation of the $S_{85}Ge_{15-x}Bi_x$ thin amorphous films system where(x = 0, 5, 10, 15, at%) was performedon two steps:

Preparation of the bulk ingots alloys
Preparation of the bulk alloys ingots started by preparing the system of powder samples to be investigated, having the composition $Se_{85}Ge_{15-x}Bi_x$, where (x = 0, 5, 10, 15 at%) from spectrally pure powder materials with 99.999 purityfrom Aldrich.
The preparation of the bulk samples was performed using the well-known melt quench technique.The differential thermal analysis DTA was performed to detect the glass forming temperature T_g, the crystallization temperature T_c, and the melting temperature T_m for each composition. (Fig.1)and (table. 1) show the DTA data for each sample.

Table [1]

Composition	T_g (°K)	T_c (°K)	T_m (°K)
Se_{85} Ge_{15}	**548.60**	**889.65**	**1074.25**
Se_{85} $Ge_{10}Bi_5$	**542.92**	**866.71**	**1005.91**
Se_{85} Ge_5 Bi_{10}	**511.99**	**841.44**	**977.12**
$Se_{85}Bi_{15}$	**491.88**	**821.08**	**903.12**

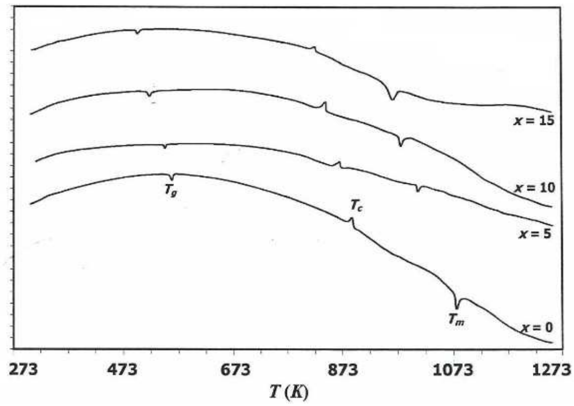

Fig. [1] DTA for bulk and the system thin films

The samples synthesis was performedin silica tubes undervacuum,(10^{-5}Torr). The tubes werewell shacked for half an hour using an electric shaker, to ensure good powder mixing and consequently homogenous alloys composition, then they were placed ina programmable furnace for 2 hours at 500 K^o, temperature was raised to 550 K^{o}for another 2 h. The temperature was increased to 1225 K^o,andkept at this temperature for 2h, then again was raised in steps each of 50 degrees up to 1373 K^o, for 10 hours. During the cooking process the tubes were frequently rockedto ensurethe homogeneity of the samples, and thenthe meltof each composition was quenched in ice water.

Preparation of the thin films
Thermal vapor deposition technique was used to form the required films by evaporating the alloys on clean quartz substrates. The films thicknesswere obtained usinga thickness monitor,Theamorphous structure of the obtained bulkmaterialsfigure (2), and the prepared thin films figure (3), were confirmed by XRD

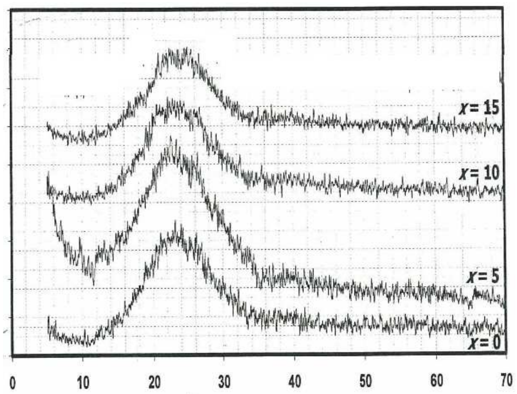

Fig. [2]

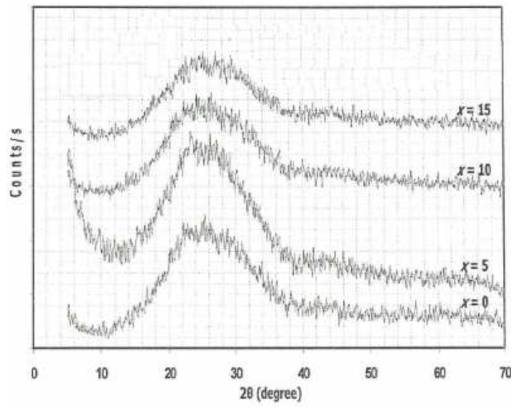

Fig. [3]

Measuring the Optical properties of the samples

Measuring Transmittance (T) and Reflectance (R)

The transmittance (T) and the reflectance (R) data were recorded at room temperature and normal incidence in the wave length range (400 – 2500 nm) using a double beam spectrophotometer type (Jasco V- 570).

The valueof T was calculated from the experimental data using the formula[(1)]

$$T = T_{exp}(1 - R_g) \quad (1)$$

Where T is the absolute value of transmittance, T_{exp} ,the experimental value, and R_g is the reflectance of the substrate.

The absolute value of reflectance R, wasdetermined using the formula

$$R = I_{rf} / I_{rM} \quad (2)$$

Where I_{rf} is the reflectance of the thin film, I_{rM} is the reflectance of the reference.

RESULT AND DISCUSSION

The Transmittance (T) and Reflectance (R), of the amorphous system, $Se_{85}Ge_{15-x}Bi_x, where\ x = 0, 5, 10, 15\ at\%$, were recorded, in the wavelength range 400 – 2500 nm. Figs.(4 - 5).

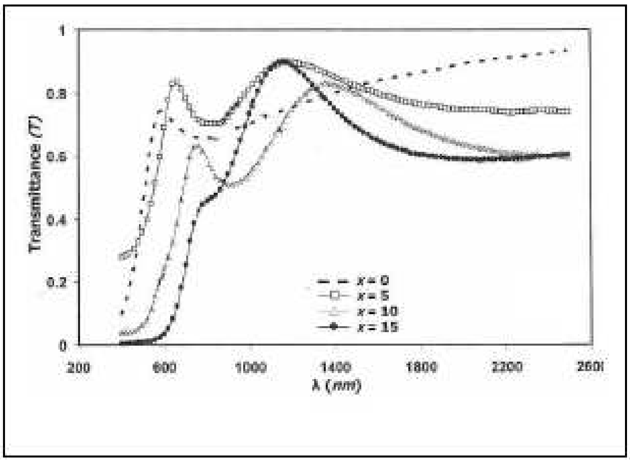

Fig. [4]

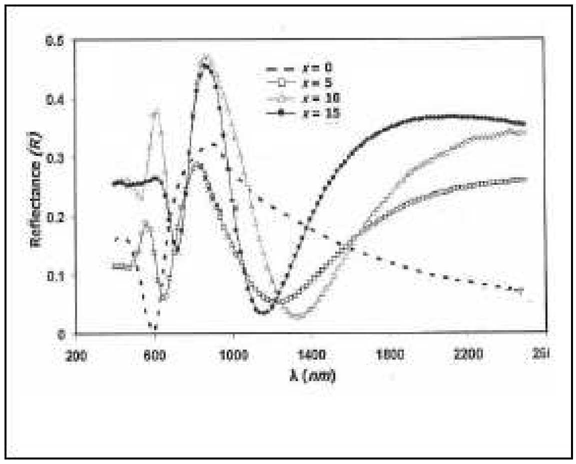

Fig. [5]

These figures illustrate that T and R, are nonlinear function at the given wavelength range. The spectral distribution of T and R revealed that the transmitted light through these materials is much more than the reflected light. This means that although each of T and R, are nonlinear function of the photons energy, the material of this system is transparent all over the light spectra in the visible and infrared regions. Also this transparency is more pronounced in the infrared region.The analysis of the results of T and R in the given spectral wavelength range, revealed that some of the light energy may be absorbed. The amount of the absorbed light energy is a good tool to study the absorption process of light through the samples of this system $Se_{85}Ge_{15-x}Bi_x$.From the obtained data of T and R , the absorption coefficient(α), for this system, could be calculated using the relation,

$$\alpha = \frac{1}{d}\left(\ln\frac{1-R}{T}\right) \quad (3)$$

Where d is the thin film thickness.

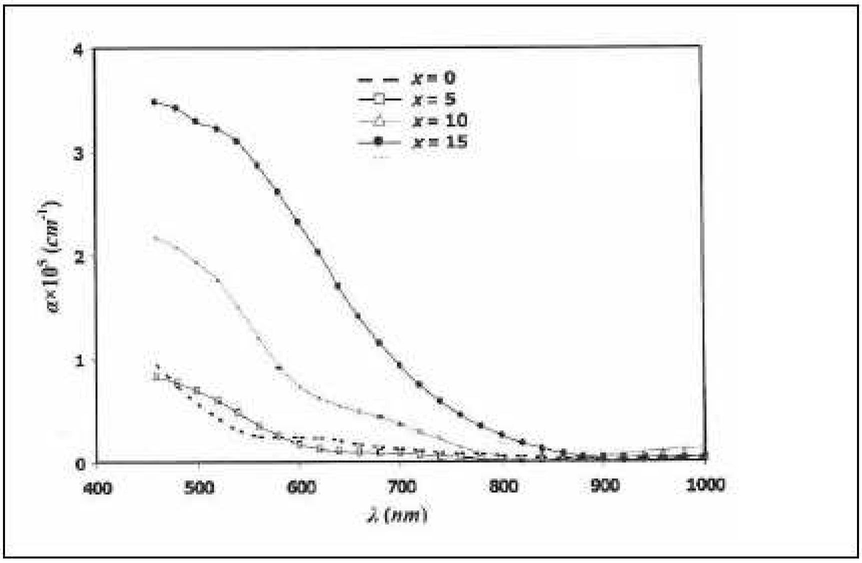

Fig. [6]

Figure (6), shows the nonlinear variation of the absorption coefficient (α), as a function of the wavelength, in the range 400-2500 nm. This figure, illustrates that the absorption coefficient has a maximum value in the ultraviolet region and decreases as the light photons energy decreases.

This result confirms the idea that this material is transparent in the visible region, and that the transparency increases as the photon energy decreases.

The obtained results for of the absorption coefficient are used to calculate the optical energy gap$(E_g^o)$for this system. In non-crystalline systems the indirect optical transition is most likely to occur(14). Under this condition the absorption coefficient is related to the photon energy by the formula(14)

$$\alpha h\upsilon = A\,(h\upsilon - E_g^o)^2, \quad (4)$$

Where, A is a constant and $h\upsilon$ is the photon energy.

The relation $(\alpha h\upsilon)^{\frac{1}{2}}$ against $h\upsilon$ is given in fig. (7).

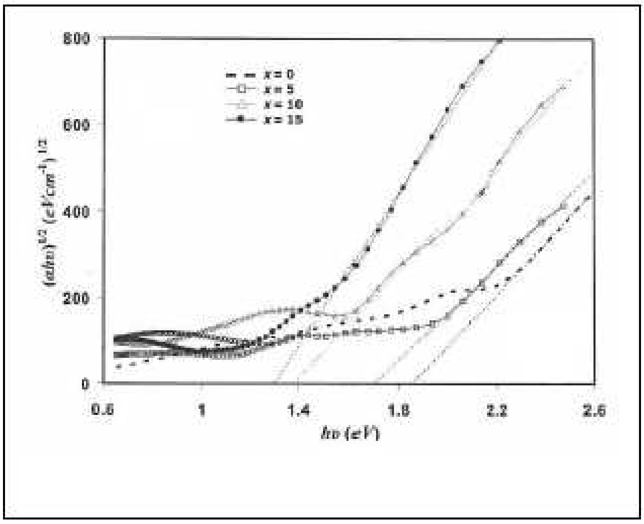

Fig. [7]

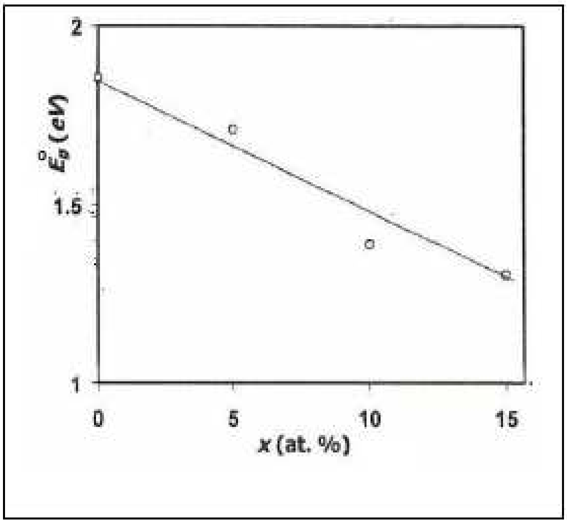

Fig. [8]

From this figure it is clear that the allowed indirect optical transition describes the transition's mechanism in this system. Also this figure shows that the absorption edge shifts towards lower photons energy as Bismuth content increases. Fig. (8), shows that the optical band gap, has been decreased as the Bismuth content increased. This may be attributed to the creation of more localized states within the energy gap as Bismuth content increases the creation of more localized states within the energy gap as Bismuth content increases [15-16].

CONCLUSION

1- The nonlinearity of the transmittance (T), reflectance (R), and the coefficient of absorption (α) as a function of the wavelength.
2- Although the thin film of this material is transparent in the visible region, it is more transparent in the infrared region.
3- The optical energy gap decreases as the bismuth content increases.
4- This material might be a good candidate for the production of high efficiency solar cells.

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