Optical absorption properties of Ge-Sb-Te films

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Received November 14, 2003

The optical properties of monolayer $Ge_2Sb_2Te_5$ thin films with three different thicknesses prepared by dc magnetron sputtering method at the range of 400 − 800 nm were studied. The optical absorption coefficients and the optical energy gap (E_g) were calculated. The results gave values for the absorption coefficients in the range of $(1.3-7.5)\times10^5$ cm^{-1} which were in the high absorption wavelength region of 400 − 800 nm. The optical energy gaps were 0.684, 0.753 and 0.810 eV corresponding the films thicknesses of 57, 88 and 127 nm, respectively, showing the characteristic of increasing with the increase of the film thickness.

OCIS codes: 310.6860, 160.4760, 210.4810.

The optical properties of amorphous solids are determined by the structural bonding between the neighboring atoms. The structural bonding in the case of chalcogens, for instance selenium and tellurium, is divalent in nature which gives rise to one-dimensional structural stability of the amorphous materials. On the other hand, the structural bonding is not highly stable[1], and chalcogens in the amorphous state have a strong tendency of crystallization. Several factors such as heat treatment, incident light, electric field, etc., are found to induce the transition. The degree of disorders and defects present in amorphous structure changes during the transition from amorphous to crystalline state[2]. Increasing disorder and defects is known to reduce the width of the optical gap shown by the model of Mott and Davis[3]. Ge-Sb-Te based materials are most suitable for high data rate optical recording. The principle underlying optical storage using phase change materials is the controlled reversible switch of a pit in the disk between two states of different reflectivity, usually amorphous and crystalline states[4]. So it is important to study the optical absorption properties of these materials for practical application.

In the present work, a systematic study of the optical absorption properties of the $Ge_2Sb_2Te_5$ amorphous thin films was made. The effect of thickness on the optical energy gap (E_g) was studied.

$Ge_2Sb_2Te_5$ thin films were deposited on 1.2-mm k9 glass substrates by dc magnetron sputtering with a $Ge_2Sb_2Te_5$ target in argon environment. The sputtering power used in this experiment was dc 150 W, and the background pressure and the sputtering pressure were 5.0×10^{-4} and 6.0×10^{-1} Pa, respectively. The thickness of films was measured by using an Alpha-Step 500 surface profilometer. Optical reflectance R and transmittance T of the films were measured using the UV/VIS/NIR spectrometer (Perkin Elmer, Lambda 900) in the wavelength range of 400 − 800 nm.

The spectral distribution of transmittance and reflectance for as-deposited $Ge_2Sb_2Te_5$ thin films of three different thicknesses are shown in Figs. 1 and 2, respectively. The results indicated that the film transmittance increased with increasing the wavelength of the incident photons and decreased with increasing the film thickness, while the reflectance increased with increasing the wavelength of the incident photons and film thickness. Taking into account multiple internal reflections[5], the optical absorption coefficient α as a function of transmittance T and reflectance R was given by

$$\alpha = (1/d)\ln\{(1-R)^2/(2T) + \{[(1-R)^2/(2T)]^2 + R^2\}^{1/2}\}, \quad (1)$$

where d is the film thickness in centimeters. In amorphous semiconductors, the optical absorption spectrum has been found to have three distinct regions[6]: the high absorption region ($\alpha \geq 10^4$ cm^{-1}), the exponential edge region ($1 \leq \alpha \leq 10^4$ cm^{-1}) and the weak absorption tail ($\alpha \leq 1$ cm^{-1}) which originates from defects and impurities.

Figure 3 shows the relation between absorption coefficient and photon energy for $Ge_2Sb_2Te_5$ thin films of three different thicknesses. The results gave values for the absorption coefficients in the range of $(1.3-7.5)\times10^5$ cm^{-1} which were in the high absorption region. In this region, the absorption coefficient of the amorphous

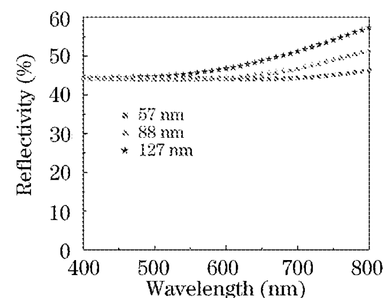

Fig. 1. Reflectance spectra of $Ge_2Sb_2Te_5$ thin films.

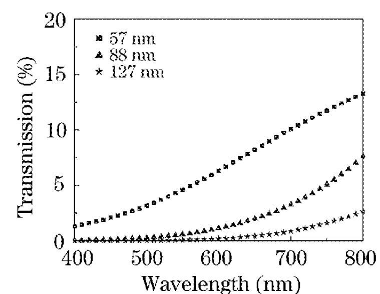

Fig. 2. Transmittance spectra of $Ge_2Sb_2Te_5$ thin films.

semiconductors follows[7]

$$\alpha hv = \mathrm{B}(hv - E_g)^n, \quad (2)$$

where B is a parameter that depends on the transition probability, hv is the photon energy, and n is an index which characterizes the transition process: $n = 1/2$ for a direct allowed transition, and $n = 2$ for an indirect allowed transition. To determine a suitable power for Eq. (2), we can substitute Y for αhv and let Y' denote the first derivative of Y with respect to photon energy, then according to Eq. (2), the ratio Y/Y' is expected to vary with hv as

$$Y/Y' = (hv - E_g)/n. \quad (3)$$

A linear relation was found to exist in all the experimental data, and the n values were obtained from the slope $(1/n)$ in the range of $1.93 - 2.03$. With reasonable approximation, the dependence of αhv on hv for the studied films could thus be considered linear with $n = 2$. The value of $n = 2$ here is reasonable as observed in other works[8−10]. The quantity $(\alpha hv)^{1/2}$ was plotted as a function of the energy of the incident photon (hv) as shown in Fig. 4. It can be seen from the figure that the experimental results show a well-defined linear region which demonstrates that Eq. (2) was satisfied with $n = 2$ in this work. The optical energy gap E_g could be obtained by intercepting with the ordinate at $\alpha hv = 0$ in the $(\alpha hv)^{1/2}$ versus (hv) plots. The values of E_g were presented in Table 1.

The experimental results show that the optical energy gap for as-deposited $Ge_2Sb_2Te_5$ thin films increase with increasing the film thickness. Similar results have been observed on many chalcogenide thin films[11,12]. Such an increase may be explained in terms of unsaturated bonds present in an amorphous materials. It is known that

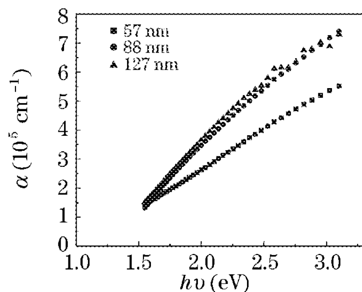

Fig. 3. Relation between absorption coefficient and photon energy for $Ge_2Sb_2Te_5$ thin films.

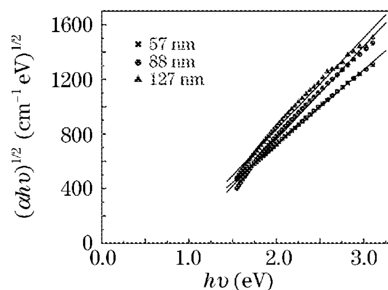

Fig. 4. The absorption coefficient plotted as $(\alpha hv)^{1/2}$ versus the photon energy (hv) for $Ge_2Sb_2Te_5$ thin films.

Table 1. Value of the Energy Gap of the As-Deposited $Ge_2Sb_2Te_5$ Thin Films with Three Different Thicknesses

Thickness (nm)	E_g (eV)
57	0.684
88	0.753
127	0.810

unsaturated bonds are produced as a result of an insufficient number of atoms deposited in the amorphous films[13]. These bonds are responsible for the formation of some defects in the films with small thickness. And according to the principle of thin film growth process[14], there should be more defects in thinner film than in thicker film. Such defects produce localized states in the band gap of amorphous solids. In the case of thicker films, greater deposition builds up more homogeneous network, minimizing the number of defects and the localized states, thereby increasing the optical energy gap.

In conclusion, the optical absorption measurements for $Ge_2Sb_2Te_5$ thin films indicated that the absorption mechanism was due to indirect transition. The absorption coefficients of $Ge_2Sb_2Te_5$ thin films were in the range of $(1.3 - 7.5) \times 10^5$ cm^{-1} which were in the high absorption region. The optical energy gap increased with increasing the film thickness.

This work was supported by the National Natural Science Foundation of China under Grant No. 60207005. M. Fang's e-mail address is fangming@mail.siom.ac.cn.

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