The Structural and Optical Properties of Hydrogenated and Nitrogenated a-Si_{0.1}Ge_{0.9} and a-Si_{0.1}Ge_{0.9}:3% B Thin Films

M. F. A. Alias

Department of Physics, College of Science, University of Baghdad, Baghdad, Iraq.

Abstract

It is shown that pure and 3% boron doped $a-Si_{0.1}Ge_{0.9}$:H and $a-Si_{0.1}Ge_{0.9}$:N thin films could be prepared by flash evaporation processes. The hydrogenation and nitrogenation are very successful in situ after depositing the films. The FT-IR analysis gave all the known absorbing bonds of hydrogen and nitrogen with Si and Ge.

Our data showed a considerable effect of annealing temperature on the structural and optical properties of the prepared films. The optical energy gap $(E_{opt.})$ of a-Si_{0.1}Ge_{0.9} samples showed to have significant increase with annealing temperature (T_a) also the refractive index and the real part of dielectric constant increases with T_a , however the extinction coefficient and imaginary part of dielectric constant decrease. The hydrogen and nitrogen alloying caused an increase in the indirect band gap($E_{opt.}$), refractive index and extinction coefficient of a-Si_{0.1}Ge_{0.9} and a-Si_{0.1}Ge_{0.9}:3% B. The boron doped films caused a decrease in $E_{opt.}$, refractive index and real part of dielectric constant while the extinction coefficient and imaginary part of dielectric constant increased.

الخصائص التركيبية والبصرية للأغشية الدقيقة المهدرجة والمنترجة Si_{0.1}Ge_{0.9} النقية والمطعمة بـ 3% بورون

ميسون فيصل الياس جامعة بغداد - كلية العلوم – قسم الفيزياء – الجادرية – بغداد – العراق

الخلاصة

تم تحضير اغشيةa-Si0.1Ge0.9:H و a-Si0.1Ge0.9:N النقية والمطعمة بالبورون بطريقة التبخير والوميضي.وتم بنجاح هدرجة ونترجة الاغشيةفي موقعها الاصلي بعد الترسيب. اعطت تحليلات FTIR اواصرالامتصاص للهيدروجين والنتروجين مع كل من السليكون والجرمانيوم كمااعطت تحليلات x-ray تركيب الاغشية المحضرة.

اوضحت النتائج ان التلدين يؤثر على الخصائص التركيبية والبصرية للاغشية المحضرة حيث ان تركيب الاغشية المحضرة حيث ان تركيب الاغشية المحضرة كان عشوائي لكل درجات حرارة التلدين ولكن فجوة الطاقة البصرية(Eopt) تزداد للاغشية غير المهدرجة او المنترجة مع زيادة درجة حرارة التلدين(Ta) وكذلك كل من معامل الاتكسار وثابت العزل الحقيقي مع زيادة Ta اينما يقل معلمل الاتكسار وثابت العزل الحقيقي مع زيادة مع زيادة الغير مباشرة بينما يقل معلمل الاتكسار وثابت العزل الحقيقي مع زيادة المعرمة المنترجة مع زيادة درجة حرارة التلدين(Ta) وكذلك كل من معامل الاتكسار وثابت العزل الحقيقي مع زيادة مع زيادة درجة حرارة التلدين(Ta) وكذلك كل من معامل الاتكسار وثابت العزل الحقيقي مع زيادة العير مباشرة بينما يقل معلمل الخمود وثابت العزل الخيالي تؤدي الهدرجة والنترجة للاغشيةزيادة في فجوة العامرة الغير مباشرة ومعامل الانكسار والخمود للاغشية النقية والمطعمة بالبورون كما ان التطعيم بالبورون ادى الى نقصان في فجوة الطاقة البصرية ومعامل الانكسار وثابت العزل الحقيقي والمعمة بالبورون كما ان التطعيم بالبورون ادى الى الخمود وثابت العزل الخيالي الحقيقي بينما تنخفض قيمة كل من معامل الانكسار والخمود الله الخصان في فجوة ومعامل الانكسار والخمود للاغشية النقية والمطعمة بالبورون كما ان التطعيم بالبورون ادى الى نقصان في فجوة الطاقة البصرية ومعامل الانكسار وثابت العزل الحقيقي بينما تنخفض قيمة كل من معامل الخمود وثابت العزل الخيالي

Introduction

In recent years a large number of researches have been working on the characteristic of tetrahedrally bonded amorphous semiconductor thin films such as hydrogenated amorphous silicon (a-Si:H). However, many of the fundamental properties of composite materials such as Si-C, Si-Ge and Si-Sn are unknown [1]. Hydrogenated amorphous silicongermanium alloys are currently attracting much interest in the development of tandem-type solar cells [2, 31. as photoreceptors for laser-beam printers using GaAlAs laser diodes [4]. SiGe semiconductors are being used to create high performance bipolar transistors. integrated circuits [5, 6], highly integrated focal-plane array infrared detectors [7], infrared light-emitting diodes [8, 9] and to be a useful optoelectronic material for wavelengths longer than $0.7 \mu m$, because of the reduction in the optical energy gap with increasing Ge content from the usual value of 1.8 eV for a-Si:H [8, 10-12].

1. Optical Absorption

Studying optical absorption, in particular the shape and shift of the absorption edge, is an extremely useful technique for understanding the basic mechanism of optically-induced transitions in crystalline and non-crystalline materials, as well as providing information about the band structure. The basic principle behind this technique is to enhance the absorption of photons with energies greater than the band-gap energy by carriers undergoing transitions from occupied states in the valence band to unoccupied states in the conduction band. Two kinds of optical transitions could occur at the fundamental edge in these materials namely direct and indirect transitions. In a direct transition the electron wave vector remains unchanged and there is no phonon interactions, while in an indirect transitions the cooperation of phonon is necessary for conserving momentum, and the electron wave vector changes.

It has been suggested by Tauc [13, 14] that the following equation may be used for calculating the absorption coefficient (α) in a direct transition:

$$\alpha (\nu) = A \frac{(h\nu - E_{opt.})^{r}}{h\nu} \dots \dots \dots (1)$$

where h is Planck constant, ν is the frequency of the incident photon, $E_{opt.}$ is the optical energy gap, A is constant depend on the density of states of film and r is the exponent which takes values of 1/2 or 3/2 depending on whether the transitions are allowed or forbidden. Tauc [14] has suggested values 2 or 3 for the r exponent which offer the best fit to optical absorption data for indirect transition in many amorphous semiconductors.

The absorption edge in semiconductors can be broadly classified into three regions (1) the weak absorption tail which originates from defects and impurities ($\alpha < 1 \text{ cm}^{-1}$) (2) Urbach edge where ($1 < \alpha < 10^4 \text{ cm}^{-1}$) according to:

(3) interband transition, but when $\alpha > 10^4$ cm⁻¹ the absorption edge is described on the basis of the indirect transition proposed by Tauc [14] as we mentioned before.

2. The Optical Constant

The optical constant parameters of solids are usually described in term of the complex dielectric function

 $\epsilon(\omega) = \epsilon_r(\omega) + i \epsilon_i(\omega)$ or the complex index of refra-ction

 $n(\omega) = n(\omega) + i k(\omega)$ and $n(\omega) = c/v$, where v in the velocity of propagation through a semiconductor and c is the speed of light, then $\varepsilon_r = n^2 - k^2$, $\varepsilon_i = 2nk$, where ε_r and ε_i the real and imaginary dielectric constant respectively. Also the optical constant of the investigated film can be completely determined from two methods (1) from spectral dependence of the transmittance (T) and absorbance (A) using the following relations [15]

$$T = \frac{(1 - R)^{2} \exp (-4 \pi k d / \lambda)}{1 - R^{2} \exp (-8 \pi k d / \lambda)}$$
.....(3)

where d is the film thickness, R is the reflectance, k is the extinction coefficient and λ is the wavelength. The absorption coefficient is related to extinction coefficient by

and the reflectance is

(2) The envelop of the transmission spectrum method [16] is customary taken to determine the points of maximum and minimum transmittance of the scan and using these extreme values to evaluate the shape of the envelop.

Manifacier et al. [17] have developed straight forward procedure for extracting refractive index, extinction coefficient from the transmission measurements provided $k^2 \ll n^2$. In this method, one constructs envelope functions T_{max} and T_{min} [16], which are treated as a continuous function of wavelength then

where

$$N = \frac{1 + n_{s}^{2}}{2} + 2 n_{s} \left(\frac{T_{max} - T_{min}}{T_{max} T_{min}} \right)$$
.....(7)

and n_s is the substrate refractive index. The reaction between the various optical constants and the details of the derivation of these relations can be seen in references [16, 17].

3. Infrared Spectroscopy

Infrared spectroscopy provides knowledge of atomic bonding modes of amorphous semiconductors which would not have become technologically suitable without hydrogen or nitrogen incorporation that reduces the defective bond density in the forbidden band gap the result of that is to allow doping in such materials and reduce the number of electronically active defect state (traps). It has been found that hydrogen or nitrogen atoms can make bonds at the defective and vacant sites to substantially remove the gap states which improves the device performance of such materials [13].

The modes of atomic motions of $Y - X_n$, where Y = Si or Ge, X = H or N and n = 1-3, where the bonding groups Y-H, $Y-H_2$ and $Y-H_3$ are designated as monohydride, dihydride and trihydride respectively. There are two types of modes (1) those involving changes in the Ge–H and Si–H bond length (stretching bond), or H–Ge–H and H–Si–H bond angle (bending bond) (2) those involving the rotation of these groups as a rigid unit (rocking, twisting or wagging modes).

IV–IV alloys such as $a-Si_xGe_{1-x}$:H or $a-Si_xGe_{1-x}$:N may be regarded as the prototypical hydrogenated or nitrogenated binary amorphous semiconductor or triary amorphous semiconductor.

The Ge– H_n groups have bonding modes in the range between 570 cm⁻¹ and 850 cm⁻¹ and the stretching modes near 1880, 1975 and 2000 cm⁻¹. The Si– H_n groups have stretching modes in the range around 2000 cm⁻¹ and bending modes near 600, 845 and 890 cm⁻¹ [18-20]. The stretching mode of the GeO group at 860 and 1860 cm⁻¹ and the stretching mode of SiOSi group at 1000 and 800 cm⁻¹ and the bending mode 450 cm⁻¹ and SiN, SiC and OH stretching modes are found between 450-1350 cm⁻¹, 830 and 3200-3400 cm⁻¹ respectively. The infrared vibrational modes in hydrogenated amorphous silicon-germanium films have been studied by many researchers [21-23]. Malinovska et al [24] have deduced from infrared spectra that hydrogen content more than 10% is a criteria of the increase Ge–H₂ and Si–H₂ absorption band, it may be due to decreasing of the density of electronic states near band edges of a-Si_{1x}Ge_x:H films. Mulato and Chambouleyron [23] and Hazra et al [25] observed absorption bond at 640 and 630 cm⁻¹ for Si–H while for Ge–H at 565 and 570 cm⁻¹ by FT-IR spectroscopy, they also estimated hydrogen bond content of a-SiGe:H thin films.

In a previous work we have prepared pure Al and As doped a-Si_{1-x}Ge_x:H thin films, with various Ge content (x = 0.3, 0.5, 0.7)and deposition temperature, by thermal evaporation technique [20]. Now the aim of the present work is to report on the influence of annealing temperature on the structural and optical properties of pure doped boron amorphous and 3% hydrogenated and nitrogenated $Si_{0,1}Ge_{0,9}$ thin films prepared by flash evaporation method.

Experimental

A polycrystalline $Si_{0.1}Ge_{0.9}$ alloy have been prepared in an evacuated quartz tube, then by flash evaporation we prepared a- $Si_{0.1}Ge_{0.9}$ thin films in vacuum about 10^{-6} mbar. The films thickness was controlled by using a quartz crystal monitor and it was about 0.4 µm. All the specimens were doped with 3.0 at %boron. Hydrogenation and nitrogenation took place in situ by exposing the a-Si_{0.1}Ge_{0.9} thin films and a- $Si_{0.1}Ge_{0.9} + 3.0\%B$ films to hydrogen or nitrogen plasma. The pure $a-Si_{0,1}Ge_{0,9}$ thin annealed films were at various temperatures within the range (298-523) K for 30 min under vacuum of 10^{-3} Torr.

The structure of the prepared films has been examined by X-ray diffraction (XRD). The composition of the alloys and thin films was determined by using X-ray fluorescence (XRF) and energy dispersive spectroscopy (EDS). The confirmation of nitrogen and hydrogen have been emphasized using Fourier transform infrared spectroscopy (FT-IR) within the wavenumber (300-2500)cm⁻¹.

The optical transmission spectrums of nitrogenated, pure and doped a-Si_{0.1}Ge_{0.9} thin films prepared on glass substrate was measured using double beam Perkin Elmer Lambda 9 (UV/VIS/NIR) spectrometer over the wavelength range 0.3 to 2.5 μ m. The transmission spectrums were used to determine the optical energy gap (E_{opt}) , Urbach energy (ΔE) and optical constant of prepared films such as refractive index, extinction coefficient as well as real and imaginary part of dielectric constant using technique envelope developed bv Swanepoel [15].

Results and Discussion

The X-ray diffraction examination of a-Si_{0.1}Ge_{0.9} thin films were carried out in order to get an idea about the structural changes produced by heat treatment at various annealing temperature with the range (298-523) K. It is observed that the prepared films have kept their amorphous structure at all the studied temperatures .The composition of Si_{0.1}Ge_{0.9} alloys and amorphous their thin films were examined by XRF and EDS to ensure the exact composition (silicon and germanium)and it is the same of the theoretical values.

The IR transmission spectrum was measured. Table (1) shows the vibration modes of a-Si_{0.1}Ge_{0.9}:H and a-Si_{0.1}Ge_{0.9}:N films. There are bond stretching mode at (2000, 2019) cm⁻¹ and (880-2000) cm⁻¹ which exhibit the Si-H and Ge-H bonds respectively and a bond bending (wagging and rocking) weak mode at 630 cm^{-1} and 600 cm⁻¹ for Si-H and strong at 560 cm⁻¹, 820 cm^{-1} , also there are absorption mode at 960 cm^{-1} for SiO, 1110 cm⁻¹ for SiN and at 770 and 860 cm⁻¹ for GeN and GeO respectively. Such results are in agreement with references [23, 26, 27].

	Vibration modes Wave number (cm) ⁻¹							
	Stretching mode	Bending mode						
GeH	1880, 2000		560, 820					
GeH ₂	1980		830					
GeH ₃	2050							
(GeH ₂) _n	1980		760, 825					
SiH	2000, 2019		600, 630					
SiH ₂	2090		580, 875					
SiH ₃	2100		862					
(SiH ₂) _n	2100		845, 890					
SiN		850, 1110						
SiO		960, 1070						
GeN		770						
GeO		860						

Table (1): Illustrate the vibration modes of hydrogenated and nitrogenated $a-Si_{0.1}Ge_{0.9}$ thin films.

We have measured the absorption coefficient of amorphous Si_{0.1}Ge_{0.9} thin films annealed at different temperatures. The influence of annealing temperature (T_a) on the absorption coefficient of a- $Si_{0.1}Ge_{0.9}$ is plotted in Fig. (1) as a function of $(\alpha E)^{0.5}$ versus E. This figure indicated that the absorption mechanism in the $a-Si_{0,1}Ge_{0,9}$ films is indirect transition. The optical absorption data also shows stabilization with annealing. By extrapolation to zero absorption, the optical energy gap has been obtained, however E_{opt} shifts towards higher photon energy with increasing T_a .The reason is that the annealing favors processes such as eliminating dangling bonds and localized states in the gap this lead to decrease the disorder of the film i.e. yields more perfect amorphous networks with increasing T_a. The shift in E_{opt} with T_a within the range (289-523) K is about 0.16 eV and E_{opt} increases monotically, with increasing T_a,

to values [0.82, 0.86, 0.91, 0.95 & 0.98] eV at [298, 373, 423, 474 & 523] K respectively.

The effect of heat treatment on the optical constant of the a-Si_{0.1}Ge_{0.9} films was studied by annealing the prepared films at various temperatures for half an hour. Fig. (2a) shows the spectral dependence of refractive index for unannealed and annealed films at different T_a. It is seen that the films refractive index increases with increasing T_a. Another noticeable remark is that n rises more rapidly with increasing wavelength (λ) from 0.8 to 1.2 then decreases moderately with μm increasing λ to 1.8 µm after that the value of n remains nearly constant for all annealed film. One can observe that the broad fundamental absorption band (peak) moves up to higher λ as T_a increases.

Fig. (2b) shows the variation of extinction coefficient (k) with λ for films annealed at

various T_a . the variation of k with λ has decreased rapidly with increasing λ from 0.8 µm to 1.2 µm after that the values became nearly constant. On the other hand the values of k decreases with increasing T_a except for the films annealed at 473 K.

Plots of the real and imaginary parts of dielectric constant versus wavelength are shown in Fig. (3a & b). We can observe that the value of ε_r increases with increasing T_a while ε_i decreases at all values of λ . On the other hand the maximum value of ε_r shifts to higher λ with increasing T_a . Another noticeable remark is that the value of ε_i decreases rapidly with increasing λ from 0.8 µm to 1.3 µm after that value the ε_i become nearly constant. Those behaviors of ε_r and ε_i with λ and T_a are look like the behavior of n and k respectively according to previous equations mentioned in (1.2).

It is interesting to observe that a strong absorption band with a maximum at about 1.1 μ m has taken place on annealing and a low-wavelength shoulder near 1.2 μ m for ϵ_{r} .

The effect of the nitrogenation and hydrogenation of pure and doped with 3.0% B amorphous $a-Si_{0.1}Ge_{0.9}$ on their optical energy gap ($a-Si_{0.1}Ge_{0.9}$, $a-Si_{0.1}Ge_{0.9}$:N, $a-Si_{0.1}Ge_{0.9}$:H, $a-Si_{0.1}Ge_{0.9}$ + 3% B, $a-Si_{0.1}Ge_{0.9}$ + 3% B:N and $a-Si_{0.1}Ge_{0.9}$ + 3% B:H) is shown in Fig. (4a, b & c).

The optical energy gap has been determined by plotting Tauc equation as mentioned before $\{(\alpha E)^{0.5}$ vs. E $\}$. One can observe that the optical absorption spectra shifts to higher photon energy for the alloys a-Si_{0.1}Ge_{0.9}:N and a-Si_{0.1}Ge_{0.9}:H films as compered to the pure i.e. the E_{opt} for pure film is 0.82 eV, for nitrogenated film is 0.92 eV and for hydrogenated film is 0.95 eV. On other hand, the decrease in E_{opt} of a-Si_{0.1}Ge_{0.9} film was about 0.10 eV after nitrogenation and 0.13 eV after hydrogenation. It has been pointed out that in general, E_{opt} increases with increasing

the amount of bonded hydrogen or nitrogen atoms [28].

The coefficient A (Tauc slope) in the eq. (1) has been obtained from the slope of the straight line in Fig. (4). The value of A of a-Si_{0.1}Ge_{0.9} thin film has increased on both nitrogenation and hydrogenation (20.25, 21.16 & 25.00) $\times 10^4$ (eV.cm⁻¹). Indeed A is known to be inversely proportional to randomness of amorphous structure and the width of the band tail [29]. Thus the increase of A value on nitrogenation and hydrogenation and hydrogenation and hydrogenation and hydrogenation and hydrogenation of pure film suggests the reduction in randomness.

The width of tail (ΔE) can be determined from the reciprocal slope of the inset of Fig. (4) which result from the equation (2) [14].Clearly the value of ΔE_0 increases when the film is hydrogenated or nitrogenated (88, 106 & 111) meV respectively. The difference between ΔE_0 for pure and hydrogenated a-Si_{0.1}Ge_{0.9} films is estimated to be about 18 meV and it is smaller than that the similar difference in case of nitrogenated i.e. 23 meV.

Fig. (5a, b & c) shows the variation of (α E)^{0.5} with photon energy (E) for a-Si_{0.1}Ge_{0.9} + 3%B:N, :H thin films. One can observe that E_{opt} increases when the doped films are nitrogenated or hydrogenated. This may indicate that alloying with nitrogen or hydrogen leads to decrease the dangling bond in the energy gap.

The inset in Fig. (5a, b & c) shows the exponential behavior in accordance with eq. (6) and the value of ΔE_0 is estimated. The increase value of ΔE_o with nitrogen or hydrogen alloying of the doped films indicates broading the band edge of the valence and conduction band on account of the narrowing of the tails ($\Delta E_0 = 105$, 118) & 115) meV. The noticeable effect observed here is that larger increases in ΔE_o and E_{opt} took place by nitrogenation than that by hydrogenation. This indicates that nitrogen incorporated in a-Si_{0.1}Ge_{0.9} is less than hydrogen. An increase in E_{opt} for $a-Si_{0.1}Ge_{0.9} + 3\%B$ films was about 0.08

eV with nitrogenation and 0.13 eV with hydrogenation and the increase in ΔE_o for doped films was about 13 meV with nitrogen and 10 meV with hydrogen. It may be not all the H-atoms have been bonded, but took place as interstitial atoms yielding states in the gap.

From figures (4 & 5 a, b, c) one can deduce that the value of E_{opt} decreases with boron doping by about 0.07 & 0.09 eV for

a-Si_{0.1}Ge_{0.9}, a-Si_{0.1}Ge_{0.9}:N and a-Si_{0.1}Ge_{0.9}:H thin films. This noticeable effect may indicate that the doping leads to an impurity states in the gap, which may visualized as decrease in the width of valence band tail leading to a shift of Fermi level towards the valence band [18]. The values of E_{opt} and ΔE_o for pure and boron doped a-Si_{0.1}Ge_{0.9}, nitrogenation and hydrogenation are tabulated in Table (2).

	<i>u 510.1000.9</i>	E _{opt} (eV)	0	and hydrogen. ΔE _o (meV)			
Thin film		Allo	ying with		Alloying with		
	Pure	N ₂	H_2	Pure	N_2	H_2	
a-Si _{0.1} Ge _{0.9}	0.82	0.92	0.95	88	111	106	
$a-Si_{0.1}Ge_{0.9} + 3\%B$	0.75	0.83	0.88	105	118	115	

Table (2): Illustrate the value of E_{opt} and ΔE_o for pure and boron doped amorphous $a-Si_{0.1}Ge_{0.9}$ alloying with nitrogen and hydrogen.

Fig. (6 a-f) shows the wavelength dependence of n and ε_r of pure and boron doped $a-Si_{0,1}Ge_{0,9}$ with and without nitrogenation or hydrogenation films. It should be pointed out that the value of n for pure film was more than its value for doped film and boron even for nitrogenated or hydrogenated films and the maximum peak of n for pure and doped films was shifted to higher wavelength i.e lower photon energy.

Another noticeable remark is that the value of n at $\lambda = 1.5 \mu m$ decrease when the film doped (this indicates a decreasing of the polarizability) and increased when the film has nitrogenated or hydrogenated, see Table (3). This is due to increase in density packing moreover the nitrogenation or hydrogenation caused to increase in the packing density and change the dangling bonds. Another noticeable remark is that the value of n decreases more rapidly when λ increases from 1.0 to 1.5 µm and then its value become constant for $\lambda > 1.5 \mu m$ for all curves.

The variation of the real part of dielectric constant with λ for pure and boron doped a-Si_{0.1}Ge_{0.9}:H and a-Si_{0.1}Ge_{0.9}:N thin films is shown in Fig. (6d, e & f). The behavior of ε_r with λ for pure and doped films is the same as that of n.

Fig. (7a, b & c) shows the variation of the extinction factor (k) as a function of λ in the range (0.8-2.4) µm for pure and boron doped $a-Si_{0,1}Ge_{0,9}$, $a-Si_{0.1}Ge_{0.9}$:H, aa-Si_{0.1}Ge_{0.9}+3%B, $Si_{0.1}Ge_{0.9}:N$, a- $Si_{0.1}Ge_{0.9}+3\%$:H and $a-Si_{0.1}Ge_{0.9}+3\%$ B:N hydrogenated and films as well as nitrogenated of these films, k is found to decrease rapidly when λ increases within 0.9 to 1.3 μ m then the value of k become constant. The value of k for pure film becomes equal to that of boron doped film when λ increase from 0.9 to 1.3 µm after that the behavior is reversed this is shown in Fig. (7a), while the behavior became apposite for $a-Si_0$ (Geo 9:H and a- $Si_{0.1}Ge_{0.9}$: N thin film as shown in Fig. (7b) & c). The increase in value of k for boron doped film is due to increase in absorption coefficient. The decrease in E_{opt} confirms such optical data.

Fig. (7d, e & f) illustrates the ε_i dependence of λ for pure and boron doped a-Si_{0.1}Ge_{0.9} films. One can observe that the variation of ε_i decreases rapidly for both films and ε_i for the pure is slightly larger than that for doped film with λ variation between 0.8 to 1.3 µm after that the value of ε_i become constant and the value of ε_i for boron doped film is more than that for pure film, these behaviors are shown in Fig. (7d), while the behavior become opposite when the pure and boron doped afilms are hydrogenated $Si_{0.1}Ge_{0.9}$ or nitrogenated for all studied values of wavelength .To give a complete picture of the data the values of n, k, ε_r and ε_i at certain wavelength (1.5) µm for pure and $a-Si_{0,1}Ge_{0,9}$ films, boron doped a- $Si_{0,1}Ge_{0,9}:N$ and $a-Si_0 Ge_0 g:H$ are tabulated in Table (3).

Table (3): The values of n, k, $\varepsilon_r \& \varepsilon_i$ for a-Si_{0.1}Ge_{0.9}, a-Si_{0.1}Ge_{0.9} + 3%B, the hydrogenation and nitrogenation films at $\lambda = 1.5 \mu m$.

Thin films n					Alloy with H ₂			Alloy with N ₂				
	n	k	٤ _r	ε _i	N	k	٤ _r	ε _i	n	k	٤ _r	ε _i
a-Si _{0.1} Ge _{0.9}	3.79	6×10 ⁻⁴	15	5×10 ⁻³	3.80	6×10 ⁻⁴	14.4	4×10 ⁻²	3.92	1.4×10 ⁻³	15.5	1×10 ⁻²
$a-Si_{0.1}Ge_{0.9} + 3\% B$	3.71	1.1×10 ⁻³	14.2	9×10 ⁻³	3.73	4×10 ⁻⁴	14.1	3×10 ⁻²	3.82	6×10 ⁻⁴	14.8	4×10 ⁻³

Conclusion

The effect of various annealing temperature, boron doped, hydrogen and nitrogen alloying on the structural and optical properties of $a-Si_{0.1}Ge_{0.9}$ thin films prepared by using flash evaporation technique were studied.

We conclude from the above work the following:

1. The increase in annealing temperature caused an increase in the optical energy gap, refractive index and real part of dielectric constant and a decrease in the extinction coefficient and imaginary part of dielectric constant.

2. The optical energy gap, refractive index and extinction coefficient increase with the nitrogen and hydrogen alloying.

3. The boron doped films causes a decrease in the optical energy gap, refractive index and real part of dielectric constant while the extinction coefficient and imaginary part of dielectric constant increased.



Fig. (1) Variation of $(\alpha E)^{0.5}$ vs. E of a-Si_{0.1}Ge_{0.9} thin films.



Fig. (2) Refractive index and extinction coefficient spectra for $a-Si_{0,1}Ge_{0,9}$ thin films.



Fig. (3) Real and imaginary part of dielectric constant spectra for $a-Si_{0.1}Ge_{0.9}$ thin films.



Fig. (4) Variation of $(\alpha E)^{0.5}$ vs. E of (a) pure a-Si_{0.1}Ge_{0.9} thin film. (b) a-Si_{0.1}Ge_{0.9}:N thin film (c) a-Si_{0.1}Ge_{0.9}:H thin film. The inset indicate ln α vs. E.



Fig. (5) Variation of $(\alpha E)^{0.5}$ vs. E of (a) pure a-Si_{0.1}Ge_{0.9} + 3% B thin film. (b) a-Si_{0.1}Ge_{0.9} + 3% B:N thin film (c) a-Si_{0.1}Ge_{0.9} + 3% B:H thin film. The inset indicate ln α vs. E.



Fig. (6) Refractive index and real part of dielectric constant of pure and doped with 3% B hydrogenated and nitrogenated a-Si_{0.1}Ge_{0.9} thin films.



Fig. (7) Extinction coefficient and imaginary part of dielectric constant of pure and doped with 3% B hydrogenated and nitrogenated a-Si_{0.1}Ge_{0.9} thin films.

References

- K. Mackenzie, J. Eggert, D. Leopold, Y, Li, S. Lin and W. Poul, Phys. Rev. B31 4 (1985) 2198.
- [2] G. Nakamura, K. Sato, Y. Yukimoto and K. Shirahata. Proc. 2nd Photovoltaic Science and Engineering Conf. Tokyo. 1980, Jpn. J. Appl. Phys. 20 Suppl. 20-2 (1981) 227.
- [3] S. Madhavi and V. Venkataraman, J. Appl. Phys. 89 (4) (2001) 2497.
- [4] S. Nishikaw, H. Kakinuma, T. Watanabe and K. Kaminishi. J. Non-Cryst. Solids 59/60 (1983) 1235.
- [5] H. Presting, in Challenges for Si-Ge Heteroepitaxy, edited by E. Fitzgerald, J. Hoyt, K. Y. Cheng, and J. Bean, MRS Symposia Proceeding No. 379 Materials Research Society, Pittsburgh (1995) 417.

- [6] B. S. Meyerson, Sci. Am. 270 (1994) 42.
- [7] B. Y. Tsaur, C. K. Chen, and S. A. Marino, Opt. Eng. 33 (1994) 72.
- [8] J. Engvall, J. Olajos, H. G. Grimmeiss, H. Prosting, H. Kibbel and E. Kasper, Appl. Phys. Lett. 63 (1993) 491.
- [9] H. Wand, M. Nagashima, K. Hayashi, J. Nakanishi, M. Kimata, N. Kumada and S. Uto, Opto-Electronics Rev. 7 (4) (1999) 305.
- [10] M. Makadsi, M. Alias and A. Al-Doori, J. Dirasat, Pure Sciences 28 1 (2001) 107.
- [11] M. Alias, H. Alamy and M. Makadsi, Renewable Energy 24 (2001) 341.
- [12] M. Alias, N. Rammo and M. Makadsi, Renewable Energy 24 (2001) 347.
- [13] Davis, E. A. and Mott, N. F., Phil. Mag. 22 (1970) 909.

- [14] Tauc, J., Grigorivicini, R. and Vancu, A., Phys Status Solidi 15 (1966) 627.
- [15] J. Pankov, "Optical Process in Semiconductors", Prentice Hall Englewood Cliffs, New Jersey (1971).
- [16] R. Swanepoel, Phys. E. Sc. Instrum. 16 (1983) 1214.
- [17] J. Manifacier, J. Gasiot and J. Fillared, J. Phys.: E. Sci. Instrum. 9 (1976) 1002.
- [18] A. Madan and M. Shaw. "The Physics and Applications of Amorphous Semiconductors", Academic Press: In New York, ed. by Madan (1986).
- [19] M. Brodsky, M. Cardona and J. Cuomo, Phys. Rev. B16 (1977) 3556.
- [20] M. F. Alias, "Optoelectronic Study of a-Si-Ge-Al (As):H Thin Films", Ph.D. Thesis, University of Baghdad (1998).

- [21] D. Malinovska, L. Nedialkova and V. Kudoyarova, Solar Ener. Mater. & Solar Cells 30 (1993) 27.
- [22] A. Middya and S. Ray, J. Appl. Phys. 75 (1994) 7340.
- [23] M. Mulato and J. Chambouleyron, Braz. J. Phys. 26 (1996) 363.
- [24] D. Malinovska, L. Nedialkova, Renewa. Ener. 5 Part III (1994) 1682.
- [25] S. Hazra, A. Middya and S. Ray, J. Non-Cryst. Solids 211 (1997) 22.
- [26] P. Wickboldt, D. Pang and W. Paul, J. Appl. Phys. 81 (1997) 6252.
- [27] J. Kleider, C. Longeaud and P. Cabarroeas, J. Non-Cryst. Solids 164-166 (1993) 403.
- [28] G. Connel and J. Pawlik, Phys. Rev. 13 (1976) 787.
- [29] N. Mott and E. Davis, Electronic Process in Non-Crystalline Materials, 2nd ed. University Press, Oxford (1979).