Structural and optical properties for nano Ga_xSb_{1-x} films

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Abstract

Alloys of Ga_xSb_{1-x} system with different Ga concentration (x=0.4, 0.5, 0.6) have been prepared in evacuated quartz tubes. The structure of the alloys were examined by X-ray diffraction analysis (XRD) and found to be polycrystalline of zincblend structure with strong crystalline orientation (220). Thin films of Ga_xSb_{1-x} system of about 1.0 μm thickness have been deposited by flash evaporation method on glass substrate at 473K substrate temperature (T_s) and under pressure 10^{-6} mbar. This study concentrated on the effect of Ga concentration (x) on some physical properties of Ga_xSb_{1-x} thin films such as structural and optical properties. The structure of prepared films for various values of x was polycrystalline. The X-ray diffraction analysis (XRD) for Ga_xSb_{1-x} showed that the preferential orientation was (111) for all values of Ga concentration. The grain size was varied with Ga concentration. The optical analysis is performed with the FT-IR spectrophotometer. The optical measurement showed that Ga_xSb_{1-x} thin films has direct energy gap .It is found that the optical energy gap increased when x increased with the range (x=0.4, 0.5 and 0.6). The optical constant for Ga_xSb_{1-x} films was varied with increasing x. These prepared polycrystalline Ga_xSb_{1-x} thin film was a good candidate for use as a base layer material in thermo photovoltaic (TPV).

Key words

Ga_xSb_{1-x} alloys and thin films, flash-evaporation, structural and optical properties.

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الخصائص التركيبية والبصرية لأغشية Ga_xSb_{1-x} النانوية

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الخلاصة

تم تحضير سبائك Ga_xSb_{1-x} بتركيز مختلفة من الكاليوم (x=0.4,0.5 and 0.6) في أنابيب الكوارتز المفرغة.تم فحص تركيب السبائك المحضرة بواسطة تحليل حيود الاشعة السينية (XRD) ووجد بأنها متعددة التبلور لتركيب zincblend باتجاهية (220). تم تحضير أغشية Ga_xSb_{1-x} بسمك واحد ميكرون بطريقة التبخير الوميضي ومرسبة على زجاج بدرجة حرارة اساس 473 كلفن وتحت ضغط 10^{-6} ملي بار. هذه الدراسة ركزت على تأثير تركيز الكاليوم (x) على بعض الخصائص الفيزيائية لأغشية Ga_xSb_1كالخصائص التركيبية والبصرية.أظهر تحليل الاشعة السينية بان اغشية Ga_xSb_{1-x} تمتلك اتجاهية(111) لجميع تركيز الكاليوم .يتغير الحجم الحبيبي مع تغير تركيز الكاليوم . تم دراسة الخواص البصرية

باستخدام مطياف FT-IR . أثبتت الخصائص البصرية ان أغشية Ga_xSb_{1-x} تمتلك فجوة طاقة مباشرة. وجد ان فجوة الطاقة البصرية تزداد بزيادة تركيز الكاليوم (0.4,0.5,0.6) .تتغير قيم الثوابت البصرية بزيادة نسبة الكاليوم (x) .جميع الاغشية المحضرة Ga_xSb_{1-x} المتعددة التبلور تعتبر مرشحا جيدا لاستخدامها كطبقة أساس في الفوتوفولتائية الحرارية (TPV) .

Introduction

The III–V compound semiconductor gallium antimonide (GaSb) has in recent years attracted much attention as an important material for fabrication infrared (IR) an optoelectronic and electronic device operated at wavelength range 1–5 μm. Antimony-based semiconducting materials are of great interest to the research and technology development for mid- and long-infrared applications. In particular, the antimony-based detector is a key component in advanced high-speed and low-noise optical receiver systems [1].

In the same line of interest, optical devices which utilize GaSb layers are important for a wide variety of optoelectronic applications, especially in thermo photovoltaic (TPV) systems. The GaSb cell is recognized as key for the development of TPV because it responds out to longer wavelengths than the silicon solar cell thus providing higher power densities in combination with heat sources. However the important problem concerning the use of GaSb in the TPV technology is the high cost of these cells, which is related to the GaSb substrates itself, the monocrystalline epitaxial layers, and the processing on the device. One possibility of reducing the wafer cost is the use of polycrystalline thin film materials and cheap substrates for the reduction of the processing cost [2**].**

GaSb has an energy bandgap of 0.70 eV(1.77 μm) at room temperature(RT) and 0.81 eV (1.53μm) at 4K. Its lattice constant of 6.0959 Å at RT matches that of various ternary and quaternary compounds with band gaps covering a wide spectral range of 0.3–1.58 eV (0.8– 4.3μm) [3].

The purpose of this paper is to investigate the effect of Ga concentration on the structural properties of prepared Ga_xSb_{1-x} alloys and films, then studied the effect x on the optical properties for prepared Ga_xSb_{1-x} films grown on glass substrates by flash-evaporation method.

Experiment

GaSb compound synthesized by using gallium whose purity is (99.999%) and antimony not less than (99.95%) then mixing a suitable atomic weight of the two elements. Putting them in evacuated sealed quartz ampoule (10^{-3} mbar) and then the sealed quartz tube heated slowly to certain temperature which was above the melting point of antimony (973 K°), gallium (578 K°) [4]. The quartz tube is kept at 1223K for 24 hour and the melting is periodically stirred to get homogenous mixture, after that the ampoule was taken out, and cooled rapidly to reduce segregation and to obtain more homogenous ingot. The structure of the ingots was characterized by XRD (Shimadzu, CuK_{α}, λ= 0.15404 nm).

Films of GaSb were deposited on thoroughly cleaned glass substrates with different concentration (x =0.4, 0.5 and 0.6) using Edwards coating system (E306A). The base pressure of the chamber was better than 1×10^{-5} mbar and the substrate temperature was 473K. In this system, vapors of the composition Ga and Sb elementary materials were sublimated through a molybdenum boat. The deposition rate was maintained at 200nm/min.

Film thickness was measured using a filmprics instrument type S20 thin film analyzer. It was *1.0 μm*. The structure of the films was characterized by XRD. The optical transmission spectra (2000-8000)

$cm^{-1}$of films were recorded by the FT-IR spectrophotometer (Shimadzu).

Results and Discussion

Figures (1 and 2) reveal the XRD patterns of Ga_xSb_{1-x} alloys and thin films with different Ga concentrations (x=0.4, 0.5 and 0.6) deposited at 473 K° substrate temperature respectively. Polycrystalline structures were presented for all prepared alloys and thin films. The XRD patterns are recorded in the range of 2θ = 10–60 ° using CuKα radiation. The thin films are dominated by three principal orientations: (111), (220) and (311).For Ga_xSb_{1-x} alloys the XRD pattern show that the zincbled structure with preferential orientation is (220) for all values of Ga concentration. One can also observe that there were unknown peaks at various 2θ as shown in Fig. (1).

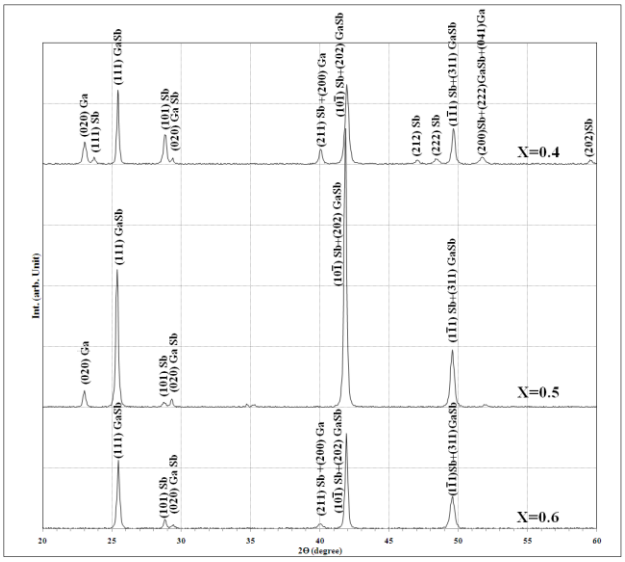

Fig. 1 XRD patterns for Ga_xSb_{1-x} alloys at different x.

Figure (2) shows the XRD patterns for Ga_xSb_{1-x} films at different concentrations suggests that all the (200) Ga_xSb_{1-x} films have highly (111) preferential orientations. Grain size is generally inferred from the relation[5]:

$$G = 0.9\lambda/\Delta(2\theta)\cos\theta \qquad (1)$$

Where G is the grain size, λ is equal to1.5404 Å, Δ (2θ) is the full width half maximum of the peak, and θ is angle of diffraction.

Grain size for prepared Ga_xSb_{1-x} alloys and films decreased with increasing of Ga concentration at preferred orientation (220) and (111) respectively as shown in the Table(1). The lattice parameter (a) of alloy and thin films was slightly varied and nearly to standard value (6.0959 Å) [3].

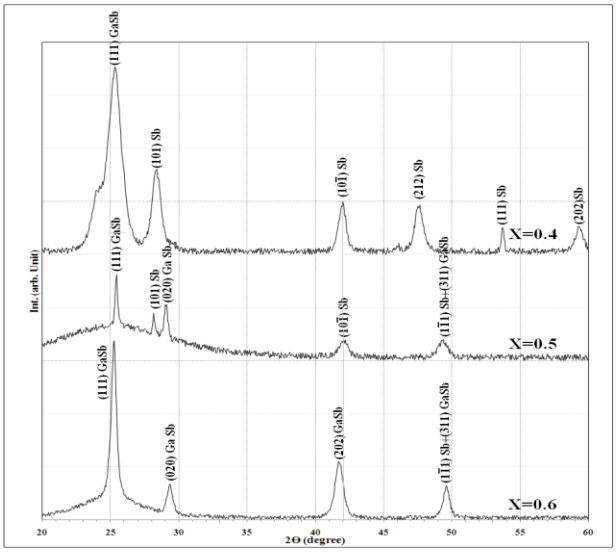

Fig. (2) XRD patterns for Ga_xSb_{1-x} films at different x.

The absorption coefficient (α) was determined from transmission spectra and the film thickness (*d*) by [6]:

$$\alpha = \frac{2.3\ log\frac{1}{T}}{d} \qquad (2)$$

The magnitude of absorption coefficient is high and is of the order of 10^4 cm^{-1}.This agrees with the bulk monocrystalline GaSb material data referred from Padiyan et al [4]. The absorption coefficient increases sharply with photon energy beyond the fundamental absorption edge. As well known, GaSb is a direct gap semiconductor for which the dependence of the absorption coefficient

on the radiation energy (*hυ)* follows Tauc relation [7]:

$\alpha h\upsilon = A\,(h\upsilon - E_g)^{1/2}$ (3)

where *h* is the Planck constant, υ is the radiation frequency, E_g is the energy band gap, and *A* is inversely proportion to amorphosity.

Table (1) Parameters of XRD Spectra for Ga_xSb_{1-x} alloys and films.

x	$2\theta°_{stan.}$	$d_{stan.}$ Å	$2\theta°_{exp}$	d (Å)	Δ (2θ)°	hkl	a(Å)	G (Å)
Ga_xSb_{1-x} alloys								
0.4			25.366	3.508	0.157	111	6.076	513
			28.776	3.099	0.179	200	6.199	505
			41.957	2.151	0.154	220	6.085	547
			49.646	1.834	0.156	311	6.085	555
0.5	25.281	3.520	25.338	3.512	0.137	111	6.083	588
	29.277	3.048						
	41.866	2.156	41.929	2.152	0.114	220	6.089	738
	49.554	1.838	49.598	1.836	0.129	311	6.090	671
0.6			25.401	3.503	0.143	111	6.068	563
			28.812	3.096	0.190	200	6.192	404
			42.029	2.148	0.155	220	6.075	543
			49.657	1.834	0.155	311	6.084	559
Ga_xSb_{1-x} films								
0.4			25.244	3.525	1.237	111	6.105	65
			8.682	3.109	0.725	200	6.219	112
			42.020	2.148	0.925	220	6.076	91
			7.954	1.895	1.150	311	6.286	75
0.5	25.281	3.520	25.352	3.510	0.646	111	6.080	125
	29.277	3.048				200	-	-
	41.866	2.156				220	-	-
	49.554	1.838				311	-	-
0.6			25.273	3.521	0.445	111	6.098	181
						200	-	
			41.969	2.150	0.540	220	6.083	156
			49.570	1.837	0.383	311	6.094	226

This relation indicates that the fundamental absorption edge of the GaSb is due to the allowed direct transitions among parabolic bands. The linear fit of $(\alpha h\upsilon)^2$ versus $h\upsilon$ allows us to obtain the value of *A* and E_g Figs.(3,4 and 5) show the variation of $(\alpha h\upsilon)^2$ versus $h\upsilon$ for Ga_xSb_{1-x} films as a function of Ga concentration to obtain the value of E_g by the extrapolation of straight line portion to α equal to zero. From these figures the values of E_g for polycrystalline Ga_xSb_{1-x} films is increased from 0.638eV to 0.675eV with increasing x from 0.40 to 0.50 then decreased to 0.619 eV with increasing x to 0.60.The increase in energy gap may be caused by decreasing in defect and localized

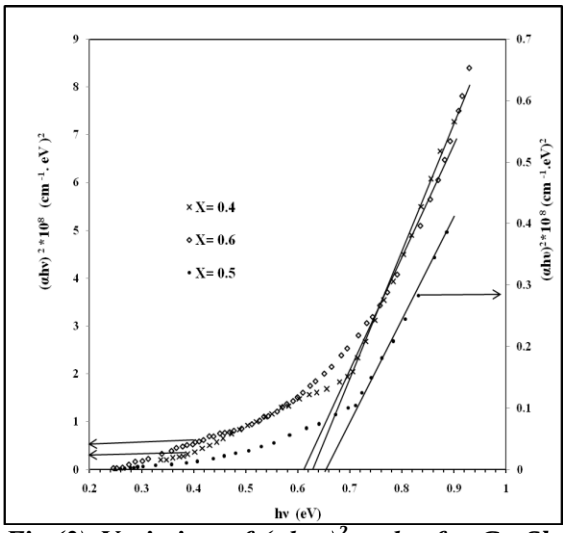

Fig.(3) Variation of $(\alpha h\upsilon)^2$ vs hυ for Ga_xSb_{1-x} films at x=0.4, 0.5 and 0.6.

Table (2) The optical parameters for Ga_xSb_{1-x} films as a function of x.

x	E_g (eV)	λ_{cutoff} (nm)	n at λ_c	k at λ_c	ε_1 at λ_c	ε_2 at λ_c
0.4	**0.638**	**1941.6**	**4.05**	**3.05**	**7.10**	**24.72**
0.5	**0.675**	**1835.4**	**2.13**	**0.64**	**4.15**	**2.73**
0.6	**0.619**	**2023.8**	**4.01**	**3.15**	**6.14**	**25.31**

states in gap in addition to its structure became nano-crystalline, while the decrease is caused by increasing in localized states This result agrees with Gheorghiu *et al* [8]. Similar behavior was shown for the refractive index (n), extinction coefficient (k), real (ε_1) and imaginary (ε_2) for dielectric constant at cutoff wavelength (λ_c).

Conclusions

The films of Ga_xSb_{1-x} have been successfully prepared by flash-evaporation method from prepared alloys on glass substrate at certain temperature. We conclude from our data that:

- The structure of prepared alloys and films are polycrystalline and have preferential orientation in the (220) and (111) direction for Ga_xSb_{1-x} alloys and films respectively.
- The grain size is varied with increasing Ga concentration for alloys and films.
- The absorption coefficient of Ga_xSb_{1-x} film is of the order of 10^4 cm^{-1}.
- The energy band gap of polycrystalline Ga_xSb_{1-x} film is increased with decreasing Sb.
- These prepared polycrystalline Ga_xSb_{1-x} film is a good candidate for use as a base layer material in TPV cells.

References

[1]F.Mohammedy, M. Deen : J. Mater Sci. Mater Electron 120 (2009)1039.

[2]Q.Zaixiang, S.Yan, H. Weiyu, H. Qing, and L.Changjian:Journal of Semi.30(2009)3.

[3]Z.Feng , F.Hou , J.Webb , Z. Shen , E. Rusli, I.Ferguson , W. Luf : Thin Solid Films 516(2008)5493.

[4]M. Hansen:Constitution of Binary Alloys, Second Edition , Mc Graw-Hill book company USA.(1958).

[5]D.Padiyan, A.Marikani,K.Murali. :Mater. Chem. and Phys.78 (2002) 51.

[6] D. Aspens, A.Studna : Phys Rev B 27 (1983) 985.

[7]J.Tauc:Amorphous and Liquid Semiconductors, New York, Plenum Press, (1974**)**.

[8]A. Gheorghiu, T. Rappeneau, J.Dupin and M.Theye: Journal de Physics (1981) C4-881.