Investigation of Optical polarizability, Absorption coefficient and Energy Gap in Al_xGa₁. _xAs Ternary Semiconductor Alloy

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Abstract:

General description of III-Arsenide Semiconductors is presented and significance of present work is stressed. The Electrical and Optical properties of III-Arsenide from binary Semiconductors are evaluated using the Principle of additivity involving quadratic expressions. The Electrical and Optical properties studied in this group include Refractive index, Optical polarizability, Absorption coefficient and Energy gap. A comparison of these data is made with reported data wherever available. The significance of present method developed from refractive indices with out need for sophisticated experimental methods is stressed. The advantage of this Group Alloys is also outlined.

Introduction`

III-Arsenide has important position in Science and Technology of Compound semiconductors in modern Electronic and Optical devices. Semiconductor alloys, which are solid solutions of two or more semiconducting elements, have important technological applications, especially in the manufacture of electronic and electro-optical devices. One of the easiest ways to change artificially the electronic and optical properties of semiconductors is by forming their alloys; it is then interesting to combine two different compounds with different optical band gaps and different rigidities in order to obtain a new material with intermediate properties. Hence the major goal in materials engineering is the ability to tune the band gap independently in order to obtain the desired properties. The zinc-blende compounds AlAs, GaAs, InAs and BAs have been arousing increasing interest, both theoretically and experimentally, because of their potentially inherent advantages. There is a considerable interest in the study of ternary alloy semiconductors such as $Al_xGa_{1-x}As$, $In_xGa_{1-x}As$ with the ultimate object of providing device materials with a specific band gap and band structure. The maximum direct energy gap requirement for solar cells, light emitting diodes and semiconductor lasers has led to the use of Al_xGa_{1-x}As alloys, where the band gap can be increased by addition of Al. The purpose of using Group-III Arsenide alloys is to obtain a material which consumes the minimum of power with maximum brightness. Liquid phase epitaxy compared with molecular beam epitaxy or metal organic chemical vapour deposition still continues being a useful technique for obtaining optoelectronic devices based on III-V Ternary compounds. The main interest of the work is the development of the III-Arsenides for applications on current quantum well technology. In this work we report the Optical and electrical characterization of $Al_xGa_{1-x}As$ epitaxial layers. [1]

Arsenides

We present a study of the Optical and Electrical properties of the AlAs, GaAs, InAs semiconductors and their alloys Al_xGa_{1-x}As, In_xGa_{1-x}As, Al_xIn_{1-x}As, InP_xAs_{1-x}, GaAs_xP_{1-x} and AlAs_xP_{1-x}. Because of the technological importance of Al_xGa_{1-x}As, its various properties have been extensively studied. In particular, parameters of the Al_xGa_{1-x}As band structure have been determined from a variety of measurements, including photo response, optical transmission and photoluminescence and variation of Hall electron concentration with temperature. We present a comprehensive up-to-date compilation of band parameters for the technologically important III-V zinc blende compound semiconductors: GaAs, AlAs and InAs along with their ternary alloys. The III–V Arsenide semiconductors are important materials in the fields of fabrication of microwave, optoelectronic, and electronic devices. The film materials of devices are usually obtained by several techniques, such as metal organic vapour phase epitaxy (MOVPE), molecular beam epitaxy (MBE) and liquid phase epitaxy (LPE). Semiconductor material selection plays a vital role in developing semiconductors. [2]

4.2.1 Al_xGa_{1-x}As

In Metal Organic Chemical Vapour Deposition (MOCVD), $Al_xGa_{1-x}As$ thin films were characterized using Raman and Hall measurements. The $Al_xGa_{1-x}As$ thin films were grown by Metal Organic Chemical Vapour Deposition (MOCVD) using metallic arsenic instead of arsine as the arsenic precursor. Some difficulties in the growth of $Al_xGa_{1-x}As$ by Metal Organic Chemical Vapour Deposition (MOCVD) are the composition homogeneity of the layers and the oxygen and carbon incorporation during the growth process. The composition homogeneity of the films was demonstrated by the Raman measurements. Hall measurements on the samples showed highly compensated material. Samples grown at temperatures lower than 750°C were highly resistive. Independently of the V/III ratio; the samples grown at higher temperatures were n-type. As the growth temperature is increased the layers compensation decreases but the Raman spectra show that the layers become more defective [3].

Method of study

The refractive index, Optical polarizability, Absorption coefficient and Energy gap of Arsenide Semiconductor alloys are evaluated by using Principle of additivity and quadratic expressions. The principle of additivity is used to study Physical properties even at very small compositions. The calculated Properties of refractive index, Optical polarizability, Absorption coefficient and Energy gap versus concentrations was fitted by equations

Method 1

 $A_{12}=A_1*x+A_2*(1-x) + 1/1000*SQRT (A_1*A_2)*x*(1-x)$

Method 2

 $A_{12}=A_1*x+A_2*(1-x)+1/1000*$ SQRT $(A_1*A_2*x*(1-x))$

Method 3

 $A_{12}=A_1*x+A_2*(1-x) - 1/1000*SQRT (A_1*A_2)*x*(1-x)$

Method 4

 $A_{12}=A_1*x+A_2*(1-x) - 1/1000*SQRT (A_1*A_2*x*(1-x))$

Additivity

$A_{12}=A_1*x+A_2*(1-x)$

Where A_{12} denotes Optical Polarizability (α_{m12}), Absorption coefficient (α_{12}) and Energy gap (Eg₁₂). A_1 and A_2 denotes Optical Polarizability (α_m), Absorption coefficient (α), Energy gap (Eg) of two binary compounds forming ternary compound.

Optical polarizability

Optical Polarizability (α_m) is used to study Optical behaviour of binary and Ternary Semiconductors belonging to III-Arsenide Ternary Semiconductor alloys.

Optical polarizability of Binary Compounds

Lorentz-Lorenz relation

The mean Optical polarizability α_M for binary semiconductors is obtained by using Lorentz-Lorenz relation [12] given below

$$\alpha_{\mathrm{m}} = \left(\frac{\mathbf{n}^2 - \mathbf{1}}{\mathbf{n}^2 + \mathbf{1}}\right) \frac{\mathsf{M}}{\rho} \quad \frac{3}{4\pi\mathsf{N}}$$

Where M, N, n, p refer to Molecular weight, Avogadro number, Refractive index and density

New dispersion principle

The equation of motion of the electron may be written as

$$mZ + mbZ + \omega_0^2 mZ = eE_0 e^{i\omega t}$$

Here $Ee^{i\omega t}$ refers to the electric force, $\omega = 2\pi v$, m is the electron mass,

 ω_0 is Natural frequency of the electron and mbZ represents the damping term.

By solving the above equation, value of z will be obtained in the form as

$$Z = \frac{(\frac{e}{m})E_0e^{i\omega t}}{\omega_0^2 - \omega^2 + i\omega b}$$

Thus the moment induced (P) per unit volume will be

$$P = \Sigma Z e$$

$$P = \frac{\nu(\frac{e^2}{m})E_0e^{i\omega t}}{\omega_0^2 - \omega^2 + i\omega b}$$

Here v is Loschmidt number

Displacement vector is obtained as

$D=E+4\pi p$

D=E+4
$$\pi \left[\frac{\nu \left(\frac{e^2}{m}\right) E_0 e^{i\omega t}}{\omega_0^2 - \omega^2 + i\omega b} \right]$$

$$D = E \left[1 + \frac{4\pi v \left(\frac{e^2}{m}\right)}{\omega_0^2 - \omega^2 + i\omega b} \right]$$
$$\frac{D}{E} = (n - ik)^2$$
$$\frac{D}{E} = \left[1 + \frac{4\pi v \left(\frac{e^2}{m}\right)}{\omega_0^2 - \omega^2 + i\omega b} \right]$$

The expression of n can be obtained by separating real and imaginary parts in above equations

i.e n=1+2
$$\pi \frac{e^2 v}{m} \frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2)^2 + \omega^2 b^2}$$

If incident frequency $\omega < \omega_0$ then $\omega^2 b^2$ can be neglected. Thus above equation can be written as

i.e n=1+
$$\frac{2\pi e^2 v}{m(\omega_0^2 - \omega^2)}$$

Rearranging the terms in above equation, we get

$$\begin{bmatrix} \frac{1}{\lambda_0^2} - \frac{1}{\lambda^2} \end{bmatrix} = \frac{e^2 \nu}{2\pi c^2 m(n-1)}$$
$$\frac{1}{\lambda^2} = \alpha + \frac{\beta}{(n-1)}$$

Optical Polarizability of binary compounds can be calculated by using new dispersion relation [13] by knowing α and β values

$$\frac{1}{\lambda^2} = \alpha + \frac{\beta}{n-1}$$

Where $\alpha = \frac{1}{\lambda 0^2}$ and $\beta = -\frac{e^2 v}{2\pi m c^2}$

Dividing through out by β and rearranging the terms n_{α}

$$\frac{1}{n-1} = \frac{1}{\beta\lambda^2} - \frac{\alpha}{\beta}$$

This equation is of the form Y=mx+c

Lt(
$$\lambda \rightarrow \infty, \frac{1}{\beta\lambda^2} \rightarrow 0$$
)
Hence $\frac{1}{n\infty - 1} = -\frac{\alpha}{\beta} = \gamma$
 $n_\infty - 1 = \frac{1}{\gamma}$
 $n_\infty = \frac{1 + \gamma}{\gamma}$

$$\frac{n_{\infty}^2 - 1}{n_{\infty}^2 + 2} = \frac{\frac{(1 + \gamma)^2}{\gamma^2} - 1}{\frac{(1 + \gamma)^2}{\gamma^2} + 2}$$

Substitute the value of $\frac{n_{\infty}^2-1}{n_{\infty}^2+2}$ in Lorentz-Lorenz formula, we get

$$\alpha_{m} = \left(\frac{(\gamma+1)^2 - \gamma^2}{(\gamma+1)^2 + 2\gamma^2} \right) \frac{\text{M}}{\rho} \quad \frac{3}{4\pi \text{N}}$$

Where M, N and ρ are molecular weight, Avogadro number and density of Binary Semiconductors and $v=-\frac{\alpha}{\beta}$

Here α is Y-Intercept and β is the slope.

Table 4.2

Compound	Optical
	Polarizability
	α _m
	$(cms)^{3}$ []
AlAs	71.14
GaAs	82.75
InAs	104.90

4.3.3 Absorption coefficient

Lorentz-Lorenz relation for solids is represented as follows

$$\left(\frac{n^2-1}{n^2+1}\right) = \frac{4\pi\nu\alpha_m}{3}$$
$$(n^2-1) = \frac{4\pi\nu\alpha_m \cdot 3}{3-4\pi\nu\alpha_m} = \left(\frac{1}{3} - \frac{1}{4\pi\nu\alpha_m}\right)^{-1}$$
$$\frac{1}{3} - \frac{1}{4\pi\nu\alpha_m} = \left(\frac{1}{n^2-1}\right)$$
$$(n^2-1) = \frac{12\pi\nu\alpha_m \cdot n}{3-4\pi\nu\alpha_m}$$

The absorption coefficient $\alpha = 2\mathbf{k} = \frac{32\pi^3}{3\nu\lambda^4}(n-1)^2$

From the above two equations we get

$$\frac{(n^2 - \mathbf{1})}{(n-1)^2} = \left(\frac{\mathbf{12}\pi\mathbf{v}\alpha_{\mathbf{m}}}{\mathbf{3} - \mathbf{4}\pi\mathbf{v}\alpha_{\mathbf{m}}}\right)^1 \frac{\mathbf{32}\pi^3}{\mathbf{3}\mathbf{v}\lambda^4\alpha}$$
$$\frac{(n^2 - \mathbf{1})}{(n-1)^2} = \mathbf{f}(\text{consider})$$

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$$\frac{n+1}{n-1} = f \text{ Or } n = \frac{f+1}{f-1}$$

$$i.e n = \left(\frac{\frac{128\pi^4 \alpha_m}{\alpha\lambda^4(3-4\pi\nu\alpha_m)}+1}{\frac{128\pi^4 \alpha_m}{\alpha\lambda^4(3-4\pi\nu\alpha_m)}-1}\right)$$

$$i.e \frac{n+1}{n-1} = \frac{128\pi^4 \alpha_m}{\alpha\lambda^4(3-4\pi\nu\alpha_m)}$$

$$Or$$

$$\alpha = \frac{128\pi^4 \alpha_m}{\alpha\lambda^4(3-4\pi\nu\alpha_m)} \left(\frac{n-1}{n+1}\right)$$

$$\alpha = \frac{128\pi^4 \alpha_m}{\alpha\lambda^4(3-4\pi\nu\alpha_m)} \left(\frac{n-1}{n+1}\right)$$

$$\alpha = \frac{128\pi^4 \alpha_m}{\alpha\lambda^4(3-4\pi\nu\alpha_m)} \left(\frac{n-1}{n+1}\right)$$

Here
$$v = \frac{N\rho}{M}$$

Where N is Avogadro number ρ is the density and M is molecular weight of the Semiconductor.

Thus the expression for absorption coefficient of binary semiconductor is given as [12]

$$\alpha = \left(\frac{128\pi^4\alpha_m}{\lambda^4}\right) \left(\frac{n-1}{n+1}\right) \left(\frac{M}{3M-4\pi N\rho\alpha_m}\right)$$

Where α_m , n, M, ρ and λ refer to the Optical Polarizability, Refractive index, molecular weight, density and wavelength of Binary semiconductors. N is Avogadro number.

Similarly for Ternary Semiconductors, the expression for absorption coefficient can be given as

$$\alpha = \left(\frac{128\pi^4\alpha_{m12}}{\lambda^4}\right) \left(\frac{n_{12}-1}{n_{12}+1}\right) \left(\frac{M_{12}}{3M_{12}-4\pi N\rho_{12}\alpha_{m12}}\right)$$

Where α_{m12} , $\mathbf{n_{12}}$, $\mathbf{M_{12}}$ and ρ_{12} are Optical Polarizability, refractive index, molecular weight and density of Ternary Semiconductor alloys and N is Avogadro number. They are calculated by using different additivity relations and Quadratic expressions [12].

4.3.4 Energy gap

The Electrical conductivity of Semiconductors depends on width of Energy Gap and it is affected by Dopant composition, Temperature, Pressure, Magnetic and Electrical fields. Indirect band gap Semiconductors is inefficient for emitting light. Semiconductors that have direct band gap are good light emitters. A wide band gap (WBG) semiconductor is a semiconductor with an energy band gap wider than about 2 eV, suitable for microwave devices. A narrow band semiconductor has energy band gap narrower than about 2 eV suitable

for tunnel devices and infrared technology. Band gap is measured by both spectroscopic and conductivity methods.

Energy gap of Ternary semiconductors

The formula used for calculation of Energy gap of ternary semiconductors are given below

$$E_{g} = \left\{ \frac{28.8}{((2^{x_{m}-x_{n}})^{2})^{\frac{1}{4}}} \left[\frac{1-\phi_{12}}{1+2\phi_{12}} \right] \right\}^{\left[\frac{x_{M}}{x_{N}} \right]^{2}}$$

Where x_M and x_N are the electro negativities of the constituent atoms of ternary semiconductor

$$\Phi_{12} = \left[\frac{4\pi\mathrm{N}}{3}\right] \left[\frac{\alpha_{\mathrm{M}_{12}}\rho_{12}}{\mathrm{M}_{12}}\right]$$

Where $\alpha_{M_{12}}$, ρ_{12} , M_{12} and N are optical polarizability, density, molecular weight and Avogadro number of ternary semiconductor Alloys.

Table 4.4

Compound	Energy gap
	Eg e.v[]
AlAs	2.95
GaAs	1.42
InAs	0.36

Results and discussion

The refractive index values of Binary Arsenide compound semiconductors are taken from reference [10] and are given in table 4.1. The refractive index values of Ternary semiconductor alloys are calculated by using different expressions of for whole composition range (0 < x < 1) and are presented in tables from. These values are compared with literature reported data [11, 12]. It is found that calculated values are in good agreement with reported values. Graphs are drawn for all these alloys by taking their composition values on x axis and Refractive index values on y axis. These graphs are given.

The refractive indices at various wavelengths for the binary semiconductors are taken from hand book of Optical constants of solids [14] are presented in table

4.25 to 4.33 along with $\frac{1}{n-1}$ and $\frac{1}{\lambda^2}$ values. The graphs drawn between $\frac{1}{n-1}$ and $\frac{1}{\lambda^2}$ for these Semiconductors are shown in figures. From these graphs intercept α values and the slope β of the straight line are determined and γ values are calculated. All these values are given from the table 4.6. The evaluated Optical Polarizabilities of Binary Semiconductors by using equation 4.8 are also from the table 4.6. The computed Optical polarizabilities by new dispersion relations are compared with reported values.

The values of Molecular weight (M), density (ρ) and refractive index (n) of the semiconductors which are required for evaluation of α_m are taken from CRC Hand book [15].

The Energy Gap values of $Al_xGa_{1-x}As$, $In_xGa_{1-x}As$, $Al_xIn_{1-x}As$, $InP_{1-x}As_x$ and $GaAs_{1-x}P_x$, are calculated by using of different Additivity Expressions and presented in tables. These values are compared with Reported data [11, 12].

Graphs are drawn for the above $Al_xGa_{1-x}As$, $In_xGa_{1-x}As$, $Al_xIn_{1-x}As$, $InP_{1-x}As_x$ and $GaAs_{1-x}P_x$ alloys with variation of Dopant compositions and are given in fig 4.4 to 4.8. Calculated values of Energy gap is taken on x axis and their composition values are taken on y axis.

The refractive indices at various wavelengths for the binary semiconductors are taken from hand book of Optical constants of solids [14] are presented in table along with $\frac{1}{n-1}$ and $\frac{1}{\lambda^2}$ values. The graphs drawn between $\frac{1}{n-1}$ and $\frac{1}{\lambda^2}$ for these Semiconductors are shown in figures. From these graphs intercept α values and the slope β of the straight line are determined and γ values are calculated. All these values are given from the table. The evaluated Optical Polarizabilities of Binary Semiconductors by using equation are also from the table. The computed Optical polarizabilities by new dispersion relations are compared with reported values.

The values of Molecular weight (M), density (ρ) and refractive index (n) of the semiconductors which are required for evaluation of α_m are taken from CRC Hand book [15].

	Λ-0.09							
Wave	1	R.I	1	Optical po	olarizability	Absorption	Ener	gy Gap
length	$\overline{\lambda^2}$	value	$\overline{n-1}$		α _m	coefficient	e.v	
λ (A ⁰)	In (10) ⁸	n		$(10)^{-2}$	$(cms)^3$	(α)		
	$(\mathbf{cms})^2$					$(10)^{-1} \mathrm{cms}^{-1}$		
4133	5.854	4.963	0.252	Calculate	Reported	4.317	Calculate	Reported
4275	5.472	4.838	0.261	<u>d</u>	82.03 [12]	3.747	<u>d</u>	1.42[]
4428	5.100	4.725	0.268	82.0		3.236	1.50	
4592	4.742	4.518	0.284			2.764		
4769	4.397	4.353	0.298			2.351		
4959	4.066	4.220	0.311			1.991		
5166	3.747	4.111	0.321			1.676		
5391	3.441	4.018	0.331			1.403		
5636	3.148	3.940	0.340			1.166		
5904	2.869	3.876	0.348			0.962		
7293	1.880	3.678	0.373			0.123		
8266	1.463	3.572	0.389			0.055		

Optical polarizability, Absorption coefficient and Energy Gap of Al_xGa_{1-x}As

Optical polarizability, Absorption coefficient and Energy Gap of Al_xGa_{1-x}As

	X=0.198									
Wave	1	R.I	1	Optical		Optical		Absorption	Energ	y Gap
length	$\overline{\lambda^2}$	Value	$\overline{n-1}$	polarizability		coefficient	e.v			
λ	$\ln{(10)^8}$	n		α _m		(α)				
	$(\mathbf{cms})^2$			$(10)^{-25}(\text{cms})^3$		$(10)^{-1} \mathrm{cms}^{-1}$				
4133	5.854	4.943	0.254	<u>Calculate</u>	Reported	2.657	Calculate	Reported		
4275	5.472	4.757	0.266	<u>d</u>	81.17	1.943	<u>d</u>	1.75[]		
4428	5.100	4.547	0.282	80.0	[12]	1.645	1.35			
4592	4.742	4.375	0.296			1.389				

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4769	4.397	4.235	0.309	1.170	
4959	4.066	4.118	0.321	0.984	
5166	3.747	4.022	0.331	0.822	
5391	3.441	3.940	0.340	0.684	
5636	3.148	3.871	0.348	0.566	
5904	2.869	3.815	0.355	0.465	
7293	1.880	3.635	0.379	0.591	
8266	1.463	3.457	0.407	0.220	
				0.193	
				0.112	

X=0.315

Wave	1	R.I	1	Optical pol	arizability	Absorption	Ener	gy Gap
length	$\overline{\lambda^2}$	Value	$\overline{n-1}$	α _m		coefficient		e.v
λ (A ⁰)	$\ln{(10)^8}$	n		$(10)^{-25}$	(cms) ³	(α)		
	$(\mathbf{cms})^2$					$(10)^{-1} \mathrm{cms}^{-1}$		
4133	5.854	4 .781	0.264	Calculated	Reported	2.604	<u>calculate</u>	Reported
4275	5.472	4.582	0.279	78.2	80.23	2.539	<u>d</u>	1.85[]
4428	5.100	4.404	0.294		[12]	2.478	1.42	
4592	4.742	4.258	0.307			2.424		
4769	4.397	4.135	0.319			2.378		
4959	4.066	4.032	0.330			2.336		
5166	3.747	3.945	0.339			2.300		
5391	3.441	3.872	0.348			2.269		
5636	3.148	3.815	0.355			2.244		
5904	2.869	3.758	0.362			2.218		
7293	1.880	3.509	0.398			2.159		
8266	1.463	3.404	0.416			2.334		

Optical polarizability, Absorption coefficient and Energy Gap of Al_xGa_{1-x}As

X	=0.419							
Wave	1	R.I	1	Optical pol	arizability	Absorption	Energ	y Gap
lengt	$\overline{\lambda^2}$	Value	$\overline{n-1}$	α _r	n	coefficient	e.v	
h	In (10) ⁸	n		$(10)^{-25}(\text{cms})^3$		(α)		
λ	$(\mathbf{cms})^2$					$(10)^{-1} \mathrm{cms}^{-1}$		
(A ⁰)					1			
4133	5.854	4.605	0.277	Calculated	Reported	2.239	Calculate	Reported
4275	5.472	4.430	0.291	79.44	79.40	1.911	1.30	1.05[]
4428	5.100	4.280	0.305		[12]	1.626		
4592	4.742	4.159	0.317			1.379		
4769	4.397	4.047	0.328			1.666		
4959	4.066	4.957	0.338			0.982		
5166	3.747	3.881	0.347			0.823		
5391	3.441	3.820	0.355			0.687		
5636	3.148	3.747	0.364			0.670		
5904	2.869	3.686	0.372			0.654		
7293	1.880	3.422	0.413			0.099		

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8266	1.463	3.341	0.427			0.090		

Optical polarizability, Absorption coefficient and Energy Gap of Al_xGa_{1-x}As X=0.491

Δ	-0.471							
Wave	1	R.I	1	Optical pol	arizability	Absorption	Energy Gap	
lengt	$\overline{\lambda^2}$	Value	$\overline{n-1}$	αι	n	coefficient	e.v	
h	In (10) ⁸	n		$(10)^{-25}$	$(\mathbf{cms})^3$	(α)		
λ	$(\mathbf{cms})^2$					$(10)^{-1} \mathrm{cms}^{-1}$		
(A ⁰)								
4133	5.854	4.483	0.287	Calculated	Reported	2.032	Calculate	Reported
4275	5.472	4.328	0.300	81.49	78.83	1.738	<u>d</u>	1.65[]
4428	5.100	4.195	0.313		[12]	1.481	1.25	
4592	4.742	4.081	0.324			1.258		
4769	4.397	3.985	0.335			1.064		
4959	4.066	3.903	0.344			0.898		
5166	3.747	3.838	0.352			0.753		
5391	3.441	3.761	0.362			0.626		
5636	3.148	3.696	0.371			0.178		
5904	2.869	3.665	0.375			0.274		
7293	1.880	3.368	0.422			0.172		
8266	1.463	3.283	0.438			0.102		

Optical polarizability, Absorption coefficient and Energy Gap of Al_xGa_{1-x}As

X=0.59

Wave	1	R.I	1	Optical pol	arizability	Absorption	Energy Gap	
lengt	$\overline{\lambda^2}$	Value	$\overline{n-1}$	α _r	$\alpha_{ m m}$		e.v	
h	In (10) ⁸	n		$(10)^{-25}$	(cms) ³	(α)		
λ	$(\mathbf{cms})^2$					$(10)^{-1} \mathrm{cms}^{-1}$		
(A ⁰)								
4133	5.854	4.343	0.299	Calculated	Reported	1.801	Calculate	Reported
4275	5.472	4.208	0.312	79.20	78.04	1.543	<u>d</u>	2.05[]
4428	5.100	4.092	0.323		[12]	1.317	2.30	
4592	4.742	3.992	0.334			1.120		
4769	4.397	3.909	0.344			0.949		
4959	4.066	3.837	0.352			0.801		
5166	3.747	3.758	0.362			0.671		
5391	3.441	3.690	0.372			0.582		
5636	3.148	3.658	0.376			0.464		
5904	2.869	3.546	0.393			0.377		
7293	1.880	3.313	0.432			0.153		
8266	1.463	3.287	0.447			0.091		

Optical polarizability, Absorption coefficient and Energy Gap of Al _x Ga _{1-x} As

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Wave	1	R.I	1	Optical pol	arizability	Absorption	Energ	gy Gap
lengt	$\overline{\lambda^2}$	Value	$\overline{n-1}$	α _r	n	coefficient	e.v	
h	In (10)	n		$(10)^{-25}$	(cms) ³	(α)		
λ	$(\mathbf{cms})^2$					$(10)^{-1} \mathrm{cms}^{-1}$		
(A ⁰)								
4133	5.854	4.196	0.313	Calculated	Reported	5.873	Calculate	Reported
4275	5.472	4.084	0.324	77.96	77.16	5.042	<u>d</u>	2.36[]
4428	5.100	3.987	0.338		[12]	4.290	2.50	
4592	4.742	3.906	0.344			3.677		
4769	4.397	3.823	0.354			3.114		
4959	4.066	3.746	0.364			2.625		
5166	3.747	3.696	0.371			2.208		
5391	3.441	3.595	0.388			1.817		
5636	3.148	3.500	0.400			1.497		
5904	2.869	3.425	0.412			1.222		
7293	1.880	3.225	0.449			0.500		
8266	1.463	3.153	0.464			0.297		

: Optical polarizability, Absorption coefficient and Energy Gap of Al_xGa_{1-x}As X = 0.804

	A-0.00							
Wave	1	R.I	1	Optical polarizability		Absorption	Energy Gap	
lengt	$\overline{\lambda^2}$	Value	$\overline{n-1}$	$\alpha_{ m m}$		coefficient	e.v	
h	In (10) ⁸	n		$(10)^{-25}(\text{cms})^3$		(α)		
λ	$(\mathbf{cms})^2$					$(10)^{-1} \mathrm{cms}^{-1}$		
$(\mathbf{A^0})$								
4133	5.854	4.050	0.328	Calculated	Reported	5.678	Calculate	Reported
4275	5.472	3.961	0.338	75.66	76.33	4.889	<u>d</u>	2.67[]
4428	5.100	3.872	0.348		[12]	4.181	2.45	
4592	4.742	3.787	0.359			3.559		
4769	4.397	3.783	0.365			3.032		
4959	4.066	3.635	0.379			2.541		
5166	3.747	3.519	0.397			2.106		
5391	3.441	3.440	0.410			1.745		
5636	3.148	3.378	0.420			1.440		
5904	2.869	3.322	0.431			0.180		

The applications of III-V Arsenide Ternary Semiconductor Alloys of $Al_xGa_{1-x}As$, as Electronic, Optical and Optoelectronic devices are determined by elementary material properties of Refractive index, Optical Polarizability, Absorption coefficient, Energy gap and Mobility. Photonic crystals, wave guides and solar cells require knowledge of refractive index and Energy gap of all above Arsenide Group alloys. The Energy gap of Semiconductor alloys determines Threshold for absorption of photons in semiconductors. Refractive index is measure of transparency of Semiconductor alloys to incident radiation. Refractive index and Energy gap of Ternary Semiconductor alloys has significant impact on Band structure. High absorption coefficient Semiconductor alloys can be used for fabricating in thin film hetero junction photovoltaic (PV) devices. Wide band gap Semiconductor alloys of $Al_xGa_{1-x}As$ are investigated for devices that allow one to attain frequencies that span over a wide range and attain Terahertz. Applications on these Ternary Semiconductor Alloy span from communications to biomedical engineering. Narrow band gap semiconductor alloys allow Hetero junction Bipolar Transistors to present terahertz (THz) operation capability. Sensors of this type exploit the unique piezoelectric, polarization characteristics, as well as the high temperature stability of wide-band gap semiconductors in order to allow stable operation with high sensitivity. Using this material system one can also explore the possibility of developing fundamental sources operating in the Terahertz regime and employing Micro-Electro Mechanical Systems (MEMS) approaches.

Recent progress and new concepts using narrow and wide-band gap Ternary semiconductor alloys of $Al_xGa_{1-x}As$, and device concepts such quantum wells with very high mobility and plasma waves will lead in Terahertz detectors and emitters. Semiconductors of this type may also be used for other novel applications such as spintronics and field emission. Terahertz signal sources based on super lattices have explored applications cover a wide range of devices, circuits and components for communications, sensors and biomedical engineering.

Research on Physical properties of III-Arsenide Semiconductor alloys is due to operating characteristics of Semiconductor devices depend critically on the physical properties of the constituent materials. The high electron mobility of InAs, is due to its narrow band gap, makes this compound useful for very high-speed and low-power electronic and infrared optoelectronic devices.

The energy band gap of Group III-V Arsenide wide Band gap Semiconductor alloys $Al_xGa_{1-x}As$ increases significantly by adding small amount of Al to GaAs, InAs and by adding As to GaP. The band gaps of these alloys are expected to vary from 1.42 ev (GaAs) to 2.67 ev (AlAs), 0.36 ev (InAs) to 2.95 ev (AlAs) and 1.42 ev (GaAs) to 2.78 ev (GaP) by increasing Al and P Concentrations. The energy band gaps of above alloys increases rapidly leading to a strong disorder when a small amount of Gallium atoms in GaAs is replaced by Al and when small amount of In atoms are replaced by Al and when small amount of As atoms are replaced by P. This occurs due to the large disparity in the electro negativity and the atomic size between Al and Ga in $Al_xGa_{1-x}As$,

The binding which was totally covalent for the elemental Semiconductors, has an ionic component in III-V Arsenide Ternary semiconductor alloys. The percentage of the ionic binding energy varies for various Semiconductor alloys. The percentage of ionic binding energy is closely related to electro negativity of the elements and varies for various compounds. The electro negativity describes affinity of electrons of the element. In a binding situation the more electro negative atoms will be more strongly bind the electron sthan its partner and therefore carry net negative charge. The difference in electro negativity of the atoms in a compound semiconductor gives first measure for Energy gap. A more electro negative element replacing a certain lattice atom will attract the electrons from the partner more strongly, become more negatively charged and thus increase the ionic part of the binding. This has nothing to do with its ability to donate electrons to conduction band or accept electrons from the valence band.

Mobility at high doping concentration is always decreased by scattering at the ionized dopants. Band gap increases with Electro negativity difference between the elements. Bond strength decreases with decrease of orbital overlapping. Large band gap in $Al_xGa_{1-x}As$, is due to high degree of orbital overlapping. Electro negativity affects the width of the band gap. Electrons

are more stabilized by more electro negativity atom. Pure semiconductors are located in Group 3 and group 4 of the periodic table. The band gaps of these materials are less influenced by electro negativity. They are influenced by configuration of crystal lattice, valence shell electrons and hybridization of orbitals.

Semiconductor Materials with higher absorption coefficients more readily absorb photons, which excite electrons into the conduction band. Knowing absorption coefficients of III-Arsenide Ternary Semiconductor alloys of $Al_xGa_{1-x}As$, aids engineers in determining which material to use in their solar cell designs. The absorption coefficient determines how far into a material light of a particular wavelength can penetrate before it is absorbed. In a material with a low absorption coefficient, light is only poorly absorbed, and if the material is thin enough, it will appear transparent to that wavelength. The absorption coefficient depends on the material and also on the wavelength of light which is being absorbed. III-V Arsenide Ternary Semiconductor Alloys have a sharp edge in their absorption coefficient, since light which has energy below the band gap does not have sufficient energy to excite an electron into the conduction band from the valence band. Consequently this light is not absorbed.

The plot of hv versus $(\alpha hv)^2$ of III-Arsenide Ternary Semiconductor alloys of Al_xGa_{1-x}As, at various concentrations of As, In, Al and P forms a straight line, it can normally be inferred that there is a direct band gap, measurable by extrapolating the straight line to the α =0 axis. On the other hand, if a plot of hv versus $\alpha hv^{1/2}$ forms a straight line, it can normally be inferred that there is an indirect band gap, measurable by extrapolating the straight line to α =0 axis. Measuring the absorption coefficient for Ternary Semiconductor Alloys gives information about the band gaps of the material. Knowledge of these band gaps is extremely important for understanding the electrical properties of a semiconductor. Measuring low values of Absorption coefficient (α) with high accuracy is photo thermal deflection spectroscopy which measures the heating of the environment which occurs when a Semiconductor sample absorbs light.

The energy levels adjust with alloy concentration, resulting in varying amount of absorption at different wavelengths in III-Arsenide Ternary Semiconductor alloys $Al_xGa_{1-x}As$. This variation in optical properties is described by the material optical constants, commonly known as Refractive index (n). The optical constants shape corresponds to the material's electronic transitions. Thus, the optical constants become a "fingerprint" for the semiconductor alloys. In $Al_xGa_{1-x}As$, the direct band gap shifts toward shorter wavelengths with increasing Al concentration.

The Optical Polarizability of Group III-V Arsenide Ternary Semiconductor alloys $Al_xGa_{1-x}As$ reduces significantly by adding a small amount of Arsenic to InP, Indium to GaAs, Al to GaAs and P to GaAs. The Optical Polarizability of these alloys are expected to vary from 102.7 (Cms)³ (InP) to 90.340 (Cms)³ (InAs) in InP_{1-x}As_x and 87 (Cms)³ (GaAs) to 75.66 (Cms)³ (InAs) by increasing As and In Concentrations. These ternary alloys are used for manufacturing infrared detectors, gas sensors.

In III-Arsenide Ternary Semiconductor alloys of $Al_xGa_{1-x}As$, replacing existing atom with high Atomic number results in Decreasing of Energy gap due to increase of charge carriers with increase of mobility and by replacing existing atoms of low atomic number result in Increase of Energy gap due to decrease of charge carriers transmitting from valence band to conduction band with decrease of mobility.

The Absorption coefficient of Group III-V Arsenide Ternary Semiconductor alloys $Al_xGa_{1-x}As$ reduces significantly by adding a small amount of Arsenic to InP, Indium to GaAs, Al to GaAs and P to GaAs. The Absorption coefficient of these alloys are expected to vary from 7.132 $(Cms)^{-1}$ (InP) to 3.012 $(Cms)^{-1}$ (InAs) in InP_{1-x}As_x and 2.298 $(Cms)^{-1}$ (GaAs) to 0.967 $(Cms)^{-1}$ (InAs) by increasing As and In Concentrations. These ternary alloys are used for manufacturing infrared detectors, gas sensors. This occurs due to the large disparity in the electro negativity and the atomic size between P and As in InP_{1-x}As_x and between In and Ga in In_xGa_{1-x}As. The Arsenic atom, Indium atom, Aluminium atom and Phosphorus atoms induces several perturbations in the host crystal

References

- 1) Puron E, Martinez-Criado G and alloys JOURNAL OF APPLIED Riech I, "Growth and Optical characterization of indirect-gap Al_xGa_{1-x}As alloys JOURNAL OF APPLIED PHYSICS VOLUME 86, NUMBER 1, 1 JULY 1999.
- 2) Adachi, S. "Physical Properties of III-V Semiconductor Compounds, "John Wiley & Sons, New York (1992)
- 3) Díaz-Reyes J" Raman and Hall characterization of AlGaAs epilayers grown by MOCVD using elemental arsenic", Superficies y Vacío15, 22-25, diciembre de ãSociedad Mexicana de Ciencia de Superficies y de Vacío-2002
- Petkov V, Jeong I, K, Mohiuddin-Jacobs F, ProffenCh and Billinge S.J.L "Local structure of In_{0.5}Ga_{0.5}As from joint high-resolution and differential pair distribution function analysis" JOURNAL OF APPLIED PHYSICS VOLUME 88, NUMBER 2 15 JULY 2000.
- 5) Catherine Priester and Genevieve Grenet, "Surface roughness and alloy stability interdependence in lattice-matched and heteroepitaxy", PHYSICAL REVIEW B VOLUME 61, NUMBER 23 15 JUNE 2000-I.
- 6) NODARKEKELIDZE, GIZOKEKELIDZE, Investigation of InP_xAs_{1-x} solid solutions and creation of the radiation-resistant materials. IPCS-2012 31^{ST} International conference on the physics of semiconductors.
- 7) Characteristics of Nitrogen-Doped GaAsP Light-Emitting Diodes, Tadashige Sato and Megumi Imai, Jpn. J. Appl. Phys. vol. 41 pp. 5995-5998 (2002)
- 8) Marius Grundmann, "The Physics of Semiconductors: An Introduction Including Nanophysics", Springer-verlag, Berlin, 2010.
- 9) D. S. Yadav, C. kumar*, J. Singh, Parashuram and G. Kumar"Optoelectronic properties of zinc blende and wurtzite structured binary solids"Journal of Engineering and Computer Innovations Vol. 3(2), pp. 26-35, March 2012
- 10) Naser M. Ahmed*, ZalimanSauli, UdaHashim, Yarub Al-Douri Investigation of the absorption coefficient, refractive index, energy band gap, and film thickness for Al_{0.11}Ga_{0.89}N, Al_{0.03}Ga_{0.97}N, and GaN by optical transmission method, Int. J. Nanoelectronics and Materials 2 (2009) 189-195.
- 11) http://www.cleanroom.byu.edu/EW_ternary.phtml-BRIGHAM YOUNG UNIVERSITY, Department of Electrical and Computer Engineering, "Direct Energy Band Gap in Ternary Semiconductors".
- 12) Sathyalatha K.C PhD Thesis"Optical and related properties of few II-VI and III-V Semiconductors" SKU University, Anantapuram (2012)
- 13) Murthy V.R, Jeevan kumar.R and Subbaiah, D.V., "New dispersion relation: Relation to ORD, MORD and Molecular Polarization' Proc viii Annual conference on IEEE/EMBS, Texas, XIV, P. 1636-1639 (1986).
- 14) Edward D. Palik, Handbook of Optical Constants of Solids, Volume 2, Academic press, 21 march 1991

- 15) William M. Haynes, David R. Lide, CRC Hand book of Physics and chemistry, Taylor & Francis Group, 91st Edition, 26-May-2010.
- 16) N.M. Ravindra, preethi Ganapathi, Jinsoo choi Energy gap-Refractive index relations in Semiconductors- An overview Department of physics, New jersey institute of technology, Newyork, USA, Infrared physics and Technology (2006).
- 17) The refractive index of $Al_xGa_{1-x}As$ below the band gap: Accurate determination and empirical modelling S. Gehrsitz, J. Appl. Phys. **87**, 7825 (2000)
- Progress in the room-temperature optical functions of semiconductors, Aleksandra B. Djurišić, Materials Science and Engineering R Reports 38, 237 (2002)
- 19) Das T D, Mondal A and Dhar S, IEE International Workshop on the Physics of Semiconductor Devices (IWPSD), 511 (2007)
- 20) Farahmand M, Garetto Cl IEEE Trans. Electron Devices 48(3), 535 (2001)
- 21) Grolik Benno, Kopp Joachim, "Optical Properties of Thin Semiconductor Films" October, 31st 2003