

EMERGING TRENDS IN TERNARY SEMICONDUCTOR ALLOYS FOR OPTOELECTRONICS

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Abstract— Ternary semiconductors formed from II–VI or III–V elements are key materials in plans to harvest energy directly from sunlight in Optoelectronic devices. In the search for low-cost alternatives to crystalline silicon, thin film Ternary semiconductor materials are commonly used, it offers advantages over silicon. It is more efficient to create an electric field at an interface among two different Semiconductor materials, known as a hetero junction. A typical polycrystalline thin film has a thin layer on top known as a “window” material if lets almost of the light through the interface to the absorbing layer. The absorbing layer has to have a high absorption to be weak in the generation of current and a suitable band gap to provide good voltage. This work shall focus on II–VI Ternary Semiconductor materials, and emphasize their potential in solar cells and highlight challenges still to be met

Keywords— Solid state physics, Crystals, Semiconductors, Alloys, Ternary Semiconductor Alloys, Physical Properties, Optoelectronics

I. INTRODUCTION

Ternary thin films of different composition were prepared by the slurry coating technique on titanium substrates. Powders of different composition synthesized in the laboratory were used for the film preparation. The films were sintered in argon atmosphere for 20 min in the temperature range 450 - 550°C. X-ray diffraction pattern of the films exhibited hexagonal structure. The optical band gap estimated from the reflectance measurements in the range 1.72 eV – 2.44 eV. Hot probe measurements indicated the films to exhibit n-type conductivity. Indium ohmic contact was vacuum evaporated on the sides of the films for in plane resistivity measurements and on the top of the film surface for cross plane resistivity measurements. Surface morphology of then films as well as the powders was studied by atomic force microscopy.

The III-V and II-VI binary semiconducting compounds, belonging to the Telluride family are considered to be very important materials for a wide spectrum of optoelectronic applications as having specific physical properties such as direct band-gap widths, high absorption coefficients in the visible and infrared part of the solar spectrum, good electrical properties (e.g. carrier mobility and lifetime) and increased capability in obtaining adjustable n- or p-type conductivity by doping. Particularly, the visible and near infrared, direct band-gaps of CdTe (1.75 eV and HgTe (2.44 eV) respectively, make them candidates for the conversion of low energy light into electricity. Moreover, homogeneous alloys formed over the entire composition range by combination of these compounds allow the production of very interesting ternary ($0 < x < 1$) systems

There is currently a great need of solid-state ultraviolet (UV) emitters for detection of chemical and biological agents as well as for general lighting. In such applications based on III-nitride wide bandgap semiconductors, conductive n-type and p-type AlGa_N or InAlGa_N alloys with high Al contents are indispensable. The use of high Al-content AlGa_N layer is also expected to increase the overall figure of merit of the AlGa_N/Ga_N HFETs due to the combined advantages of enhanced band offset, lattice mismatch-induced piezoelectric effect, and the electron velocity in the two dimensional electron gas (2DEG) channel. Thus improving the material quality of high Al content AlGa_N alloys is also of crucial importance for fabricating high performance AlGa_N/Ga_N HFETs.

This work explains recent advances in III-V and II-VI Ternary Semiconductor Alloys. Current work has significant potential for low-cost, scalable solar cells. The close interplay among the properties of the materials and their utility in solar cells is also briefly discussed. Almost group II–VI materials are direct band gap semiconductors with high optical absorption and emission coefficients. Semiconductors of Group II-V and II–VI materials are good candidates for use in solar cells. The Electrical and Optical Properties of III-V and II-VI Ternary Semiconductor Alloys from Binary Semiconductor Alloys are derived using Additivity rule with Quadratic expressions. The Electrical and Optical Properties studied in this group are confined to Refractive index, Optical Polarizability, Absorption coefficient and Energy gap. A comparison of these data is made with reported data available. Merits of study of this group alloys is also outlined. [1]

The various applications of III-V and II-VI Semiconductor Alloys 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.

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 A system (MEMS) approaches.

Recent progress and new concepts using narrow and wide-band gap Ternary semiconductor alloys 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

The refractive index, Optical polarizability, Absorption coefficient and Energy gap of Ternary 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

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

Method 2

$$A_{12}=A_1*x+A_2*(1-x) + 1/1000* SQRT (A_1*A_2)*x*(1-x) \quad (2)$$

Method 3

$$A_{12}=A_1*x+A_2*(1-x) - 1/1000*SQRT (A_1*A_2)*x*(1-x) \quad (3)$$

Method 4

$$A_{12}=A_1*x+A_2*(1-x) - 1/1000*SQRT (A_1*A_2)*x*(1-x) \quad (4)$$

Additivity

$$A_{12}=A_1*x+A_2*(1-x) \quad (5)$$

Where A_{12} denotes Refractive index (n_{12}), Optical Polarizability (α_{m12}), Absorption coefficient (α_{12}) and Energy gap (E_{g12}). A_1 and A_2 denotes Refractive index (n), Optical Polarizability (α_m), Absorption coefficient (α), Energy gap (E_g) of two binary compounds forming ternary compound.

II. RESULTS

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. 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].

Table 1: Optical polarizability, Absorption coefficient and Energy Gap of Cd_xHg_{1-x}Te X=0.00

Wave length λ (Å) *10	$\frac{1}{\lambda^2}$ In (10) ⁸ (cms) ²	RI value n[14]	$\frac{1}{n-1}$	Optical polarizability α_m ([10]) ⁻²⁵ (cms) ³		Absorption coefficient (α) ([10]) ⁻¹ cms ⁻¹		Energy Gap E_g	
				Calculate	Reported	Calculat	Report	Calculat	Reported
4133	5.834	2.664	0.601	Calculate	Reported	Calculate	Report	Calculat	Reported
4158	5.784	2.678	0.596	107	105.4[12]	2.44	2.00	1.50	1.42[8]
4235	5.576	2.727	0.579	108		2.40	[14]		1.9[12]
4315	5.371	2.790	0.559	110		2.30			
4370	5.236	2.844	0.542	111		2.21			
4426	5.105	2.908	0.524	113		2.14			
4543	4.845	3.036	0.486	115		2.10			
4699	4.529	3.175	0.459	118		2.01			
4900	4.165	3.239	0.447	121		1.83			
5120	3.815	3.279	0.439	122		1.59			
5277	3.591	3.313	0.432	123		1.35			
5488	3.320	3.382	0.419	124		1.21			
5765	3.009	3.586	0.387	128		1.05			
						1.01			

Table7.02: Optical polarizability, Absorption coefficient and Energy Gap of Cd_xHg_{1-x}Te X=1.00

Wave length λ [Å]	$\frac{1}{\lambda^2}$ [10 ⁸ (cm) ⁻²]	R.I Value n	$\frac{1}{n-1}$	Optical polarizability α_m [10] ⁻²⁵ (cm) ³		Absorption coefficient α [10] ⁻¹ cm ⁻¹		Energy Gap E_g	
				Calculated	Report	Calculated	Report	Calculated	Reported
4133	5.854	4.050	0.328	75.66	76.33	5.67	4.5	2.45	2.67[8]
4275	5.472	3.961	0.338		[12]	4.88	[15]		
4428	5.100	3.872	0.348			4.18			
4592	4.742	3.787	0.359			3.55			
4769	4.397	3.783	0.365			3.03			
4959	4.066	3.635	0.379			2.54			
5166	3.747	3.519	0.397			2.10			
5391	3.441	3.440	0.410			1.74			
5636	3.148	3.378	0.420			1.44			
5904	2.869	3.322	0.431			0.18			

Also optical Polarizability of Cd_xHg_{1-x}Te decreases from 82.03 to 75.66 by adding small amount of cadmium with low electro negativity and low atomic number than host element mercury due to less electron stabilisation in the bonding

The binding which was totally covalent for the elemental Semiconductors, has an ionic component in II-VI 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 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. 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. Electrons are more stabilized by more electro negativity atom. An atom's electro negativity is affected by both its atomic number and the distance that its valence electrons reside from the charged nucleus. The higher the associated electro negativity number, the more an element or compound attracts electrons towards it [23].

We have investigated the MOCVD growth of III-V and II-VI Ternary Semiconductor Alloys and in

Al_xGa_{1-x}N alloys by Si-doping [18]. By examining the electrical and optical properties of vast numbers of AlGaN samples grown under different conditions, we concluded that:

(i) the conductivity of Al_xGa_{1-x}N alloys continuously

in-creses with an increase of Si doping level for a fixed value of Al content and

(ii) there exists a critical Si-dopant concentration of about

$1 \times 10^{18} \text{ cm}^{-3}$ that is needed to convert insulating Al_xGa_{1-x}N alloys with high Al contents ($x \geq 0.4$) to n-type.

This is illustrated in which shows the free electron concentration (n), mobility (μ), conductivity (I) of Si-doped Al_xGa_{1-x}N alloys as functions of the Si dopant concentration (NSi) for three different Al compositions, $x = 0.4, 0.45, \text{ and } 0.5$. The results clearly reveal that there exists a critical Si-dopant concentration for converting insulating Al_xGa_{1-x}N ($x \geq 0.4$) to n-type

Ternary Semiconductor Materials with higher absorption coefficients more readily absorbs photons, which excite electrons into the conduction band. Knowing absorption coefficients of II-VI Ternary Semiconductor alloys of Cd_xHg_{1-x}Te, 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 and II-VI 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.

In III-V Ternary thin film alloys and epitaxial layers (1 μm thick) were grown on sapphire (0001) substrates with binary buffer layers by metal organic chemical vapour deposition (MOCVD). The growth temperature and pressure were around 1050°C and 50 Torr, respectively. The metal organic sources used were trimethylgallium (TMGa) for Ga and trimethylaluminum (TMAI) for Al. For Mg-doping of AlGaN, bis-cyclopentadienyl-magnesium (Cp2Mg) was transported into the growth chamber with ammonia during growth. The gas sources used were blue ammonia (NH3) for N and Silane (SiH4) for Si doping and the doping level was varied by controlling the SiH4 flow rate. The Al contents of Ternary thin films of Al_xGa_{1-x}N alloys were determined by energy dispersive x-ray (EDX) microanalysis and x-ray diffraction (XRD) measurement as well as by the flow rates of TMGa and TMAI. The Al contents (x) determined by all three methods agreed within ± 0.02 . The Si-dopant

concentrations were determined by the flow rate of SiH₄ as well as by the variable temperature Hall effect measurement at elevated temperatures ($T < 650$ K).

Additionally, secondary ion mass spectroscopy (SIMS) measurements were performed (by Charles and Evan) for selective samples to verify the Si-dopant concentrations. Atomic force microscopy (AFM) and scanning electron microscopy (SEM) were employed to examine the surfaces and revealed crack-free Al_xGa_{1-x}N epitaxial layers. Variable temperature Hall-effect (standard Van der Pauw) measurements were employed to measure the electron concentration, mobility, and resistivity of these materials.

In II-VI Ternary Semiconductor alloys The plot of $h\nu$ versus $(\alpha h\nu)^2$ of II-VI Ternary Semiconductor alloys of Cd_xHg_{1-x}Te at various concentrations of Cd forms a straight line, it can normally be inferred that there is a direct band gap, measurable by extrapolating the straight line to the $\alpha=0$ axis. On the other hand, if a plot of $h\nu$ versus $\alpha h\nu/2$ forms a straight line, it can normally be inferred that there is an indirect band gap, measurable by extrapolating the straight line to $\alpha=0$ 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 difference in electro negativity of the atoms in III-V and II-VI compound semiconductor alloys of Cd_xHg_{1-x}Te therefore gives a first measure for Polarization. Doping is still achieved by introducing specific atoms as substitution impurities but in contrast to elemental semiconductors, we now have more possibilities.

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 semiconductor devices. Extensive research in materials has produced a number of compound semiconductors. [2]

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