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RELATIONSHIP BETWEEN THE OPTICAL BAND GAP AND MOLE FRACTION OF SOME SYNTHETIC TERNARY HETEROSTRUCTURES SYSTEMS

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ABSTRACT

Solar-blind ultraviolet photodetectors find uses in numerous applications in the defense, commercial, and scientific arenas such as covert space-to-space communications, early missile threat detection, chemical threat detection, biological threat detection, spectroscopy, flame detection and monitoring, UV environmental monitoring, and UV astronomy. The optical band gaps of six tenary heterostructures CdZnS, ZnCdTe, AlGaN, AlGaAs, InGaAs and GaAlP at 0k, 300k and 600k representing low temperature, room temperature and high temperature respectively were considered. The optical band gap changes as we varied the composition (x) of the semiconductor. The optical band gap increases with mole fraction for CdZnS, ZnCdTe, AlGaN, AlGaAs and AlGaP while it decreases for InGaAs. Since the energy gap decreases with temperature, it then follows that the optical band gap should also falls (Casey et al, 1978). AlGaN is very useful as solar-blind deep ultraviolet photodector due to its widest range of optical band gap. Solar blind UV detectors of ternary heterostructures operating in the range 240-285nm, corresponding to optical band gap Eg = 5.1767eV-4.3593eV are considered.

I. INTRODUCTION

Solar-blind deep-ultraviolet (DUV) photodetectors with excellent thermal stability have attracted a strong interest due to their broad potential applications in the fields of automatization, short-range communications security, biological researches, and military services. Solar blind photodetectors fabricated from various wide-bandgap materials, such as Al*x*Ga1−*x*N (Collins et al, 2006), diamond (Koide et al, 2002), and II–IV compounds (Sou et al, 2001), have been reported.

In the past few years, technological and scientific advances in wide bandgap AlGaN based semiconductor materials have led to a renewed interest in AlGaN based UV detectors. The AlGaN material system has a wide direct bandgap and is ideally suited to detection of UV light in the solar blind range,

Several optical studies such as Kawamural et al., (1985 a, b), peng et al., (1986), penna et al., (1985), People et al., (1983), Shum et al., (1986), Skolnick et al., (1986), weiner et al., (1985), Welch et al., (1983 a, b,1984) among other, have been carried out, whose results were interpreted using single-quantum well model?(although, could not give quantitative information about the absorption coefficient).

Adelabu et al., (1988), presented optical abosorption data between room temperature and about 100K of Ga0.47 In0.52As/A10.48 In 0.53As multiple quantum well(MQW) structures of 50Å well samples with different numbers(10,20 and 50) of wells and of two different substrate natures, namely, doped and updoped.

Optical properties of heterostructures are put to wide practical use, ranging from photodiodes detector, solar cells, lasers, and modulator (Chuang 1995).

The optical properties of superlattices (SL) and multiple quantum well (MQW) structures are considered to be determined among other variables by the band-gap difference ΔEg.

The A1GaN for example enable us to know the concentration of A1 in the heterostructure as well as the optical frequency of the illuminating source.

Another optical properties of heterostructure is optical absorption which create an election and hole. The interation between these oppositely charged particles leads to a bound state called excition (Awodugba et al., 2002).
These excition modify the strength of optical absorption strongly near the band gap. (Davies 1998). A1GaN p-i-n heterostructure is useful as a "solar – blind" detector (Brown et al., 2000 a) while visible – blind UV detectors and detector arrays based on III- V nitride structure have been reported in recent publication like Harid (1999), Brown et al., (1999, 2000a, 2000b, 2000c) and Walker et al., (2000).
By using lattice- matched multilayers of heterostructures, the band-gap of the absorbing region can be tailored to match the wavelength of the light being detected.
For example, InGaAs with an in mole fraction of 0.53 can be grown epitaxially on InP with excellent lattice matching.
This composition of InGaAs has a band gap of about 0.75 eV, which is sensitive to a useful wavelength for fiber optic systems (1.55:m) where they have minimum loss and fairly high threshold currents. (Beng1989)
In this paper we report the variation in optical band – gap of A1GaN, InGaAs, and A1InAs heterostructures with mole – fraction.

II. COMPUTATION, RESULTS AND DISCUSSION

The optical band gap Eg (x) of the tenary heterostructures AxB1-xC may be expressed (Koide et al., 1987) as: $Eg(x)=Eg(BC)(1-X)+Eg(AC)x-b(1-x)$…….. 1
Where Eg(x) is the band –gap of the compound BC and Eg(AC) that of compound AC. B is the bowing parameter which is assumed equal to 1.0eV (Shuji et al, 1997). The above equation (1) when applied to these heterostructure at 300k gives

$Eg(x)_{(AlGaN)} = Eg(1-X)_{(GaN)} + Eg(x)_{(AlN)} - b(1-x)$……..2
$Eg(x)_{(InGaAs)} = Eg(1-X)_{(GaAs)} + Eg(x)_{(InAs)} - b(1-x)$…….3
$Eg(x)_{(GaAlP)} = Eg(1-X)_{(AlP)} + Eg(x)_{(GaP)} - b(1-x)$…….4
$Eg(x)_{(AlGaAs)} = Eg(1-X)_{(GaAs)} + Eg(x)_{(AlAs)} - b(1-x)$……5
$Eg(x)_{(CdZnS)} = Eg(1-X)_{(CdS)} + Eg(x)_{(ZnS)} - b(1-x)$……6
$Eg(x)_{(ZnCdTe)} = Eg(1-X)_{(CdTe)} + Eg(x)_{(ZnTe)} - b(1-x)$……7

The band gap of GaN, AlN, GaAs, InAs, , AlAs, CdS, ZnS, CdTe, ZnTe, GaP and AlP at 0k and 300k were given by Lide (1988), Madelung (1996), (Awodugba et al, 2012), (Adelabu et al, 2004) and Adachi (1985), while their values at higher temperature 600k are deduced using the expression, (Casey et al, 1978).

$Eg(T) = Eg(0) - \frac{5.405\ X\ 10^{-4}T^2}{(204+T)}$ and are tabulated in table 1.

	Compound	Eg (0k)eV	Eg (300k)eV	Eg (600k)eV
1	GaN	3.50	3.41	3.26
2	AlN	6.30	6.20	6.06
3	GaAs	1.52	1.42	1.28
4	InAs	0.42	0.35	0.18
5	AlAs	2.23	2.15	1.99
6	CdS	2.64	2.53	2.39
7	ZnS	3.90	3.72	3.65
8	GaP	2.32	2.25	2.05
9	AlP	2.53	2.42	2.21
10	CdTe	1.61	1.50	1.36
11	ZnTe	2.39	2.20	2.14

With table 1 and computer program in pascal, the optical gaps expressed in equations (2), (3), (4), (5), (6) and (7) were computed for 100 iterations, at temperatures 0k, 300k and 600k with various values

of x, the mole fraction, in steps of 0.01, from 0 to 1.0. The results are as shown in the three plots below.

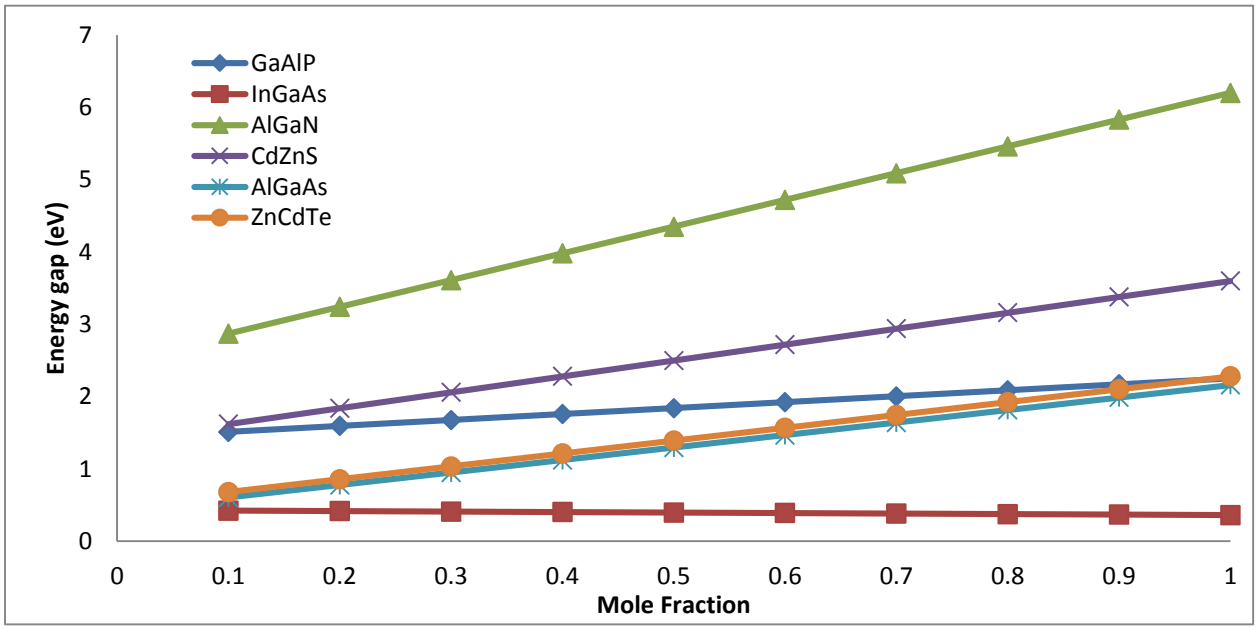

Figure 1: Optical-Band gap variation of ternary heterostructures at 300k

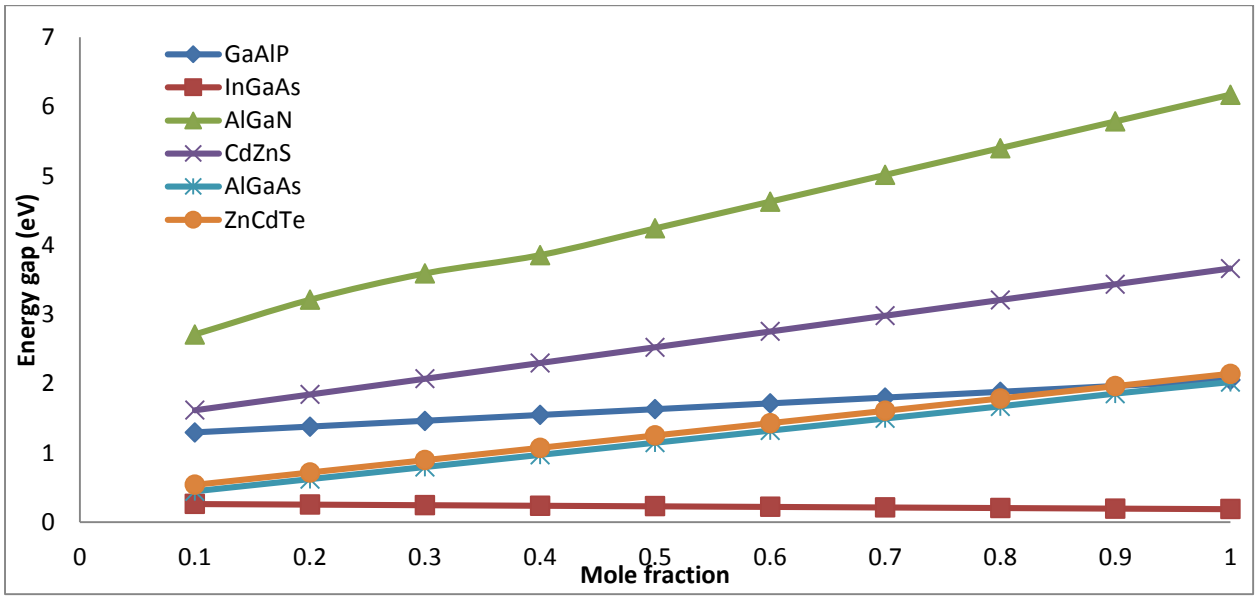

Figure 2: Optical-Band gap at 300k

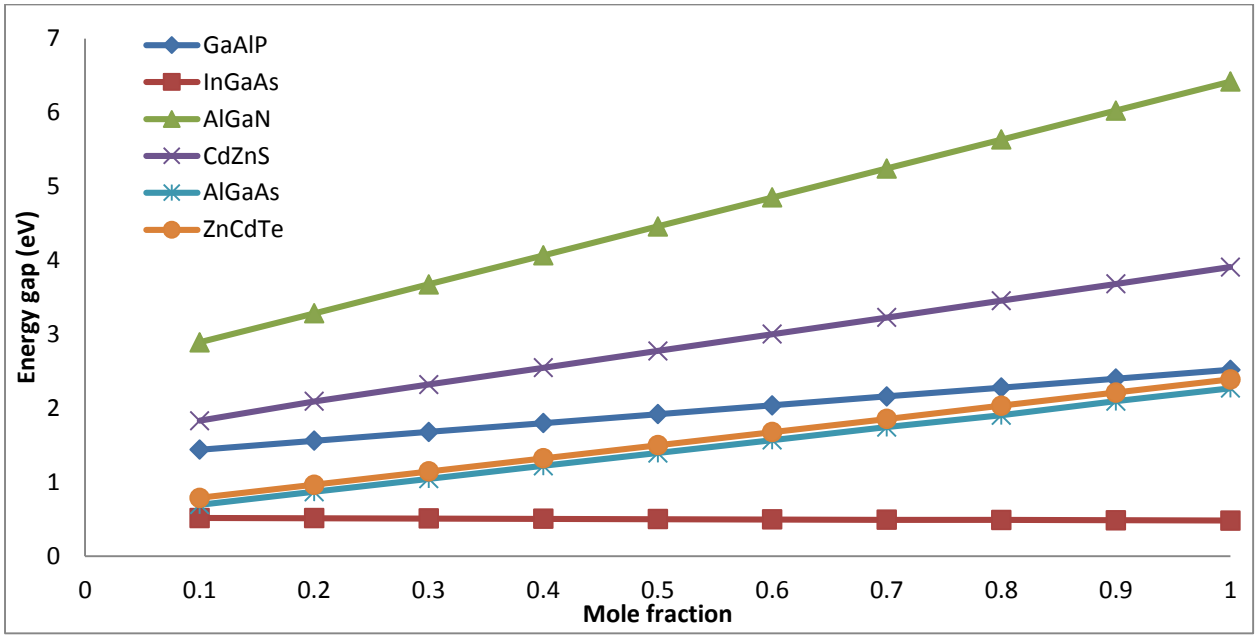

Figure 3: Optical band gap at 0k

Six ternary heterostructures were examine of which $Al_xGa_{1-x}N$ was found to be useful as solar blind detector in the mole fractions 0.5, 0.6 and 0.7 with corresponding band gap 4.35ev, 4.72eV and 5.09eV at 0k. The mole fraction of solar blind AlGaN at 300k are 0.6 and 0.7 with corresponding band gaps 4.63eV and 5.012eV. At 600k, the mole fraction are 0.5, 0.6 and 0.7 with corresponding wavelength 4.46eV, 4.86eV and 5.15eV. The high energy band gap of the AlGaN alows it to be useful for various scientific and technological applications such covert communication (Chen et al, 2009), astronomical imaging (Clarck et al, 1999), chemical sensing (Hudeish et al, 2003), detection of flame and electric discharge (Oshimal et al, 2009) and early missile warning (Hudeish et al, 2003)

III. CONCLUSION

The optical band gaps of the six tenary heterostructures at 0k, 300k and 600k representing low temperature, room temperature and high temperature respectively followed the same trend. It increases with mole fraction, x for AlGaN, GaAlP, AlGaAs, ZnCdTe, and CdZnS, while it decreases for InGaAs. The reason for this trend may be attribute to choice of the bowing factor,b, for the six heterostructures. While (Shuji et al, 1997) assumed a bowing factor of 1.0eV for AlGaN, which gave a satisfactory result that is in conformity with existing fact, it is not true for InGaAs, which gave a result that negates the existing fact. As a result, there is a need to find appropriate bowing factor for InGaAs, and many other tenary hetestructures. Since energy gap of a semiconductor decreases with temperature, it then follows that the optical band gap should also falls (Cassey et al, 1978). This is the case for the six tenary heterostructure considered.

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