TEMPERATURE DEPENDENCE OF EFFECTIVE BAND GAP, REFRACTIVE INDEX, DIELECTRIC FUNCTION AND MODEL PARAMETERS C(x,T), A(x,T) of $AlXGa_{1-X}N$.

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Abstract: The Refractive Index and Effective Band Gap variation of wurzite $Al_XGa_{1-X}N$ with respect to temperature with bowing parameter b=1.3±0.2 eV, have been studied. Refractive index found to increase for all compositions and its rate of increase is more in the vicinity of band gap. A set of values for model parameters C(x, T) and A(x, T) were obtained for different compositions and temperatures. The variations of C(x, T) and A(x, T) with compositions were found to be stronger than their corresponding temperature variations. The variation in dielectric function expressed in terms of C(x, T) and A(x, T) with respect to temperature and composition have been studied. It is found that dielectric function is nonlinearly increasing with increasing temperature and composition. This work enables us to calculate refractive index of GaN and AlGaN alloys at any desired temperature and hence to predict properties of GaN based waveguides at elevated temperatures.

***IndexTerms* - Laser diode, Waveguide, Temperature drift, Effective band gap (EBG), Dielectric function.**

I. INTRODUCTION

The III-V nitride materials are having potential optoelectronic applications in blue and UV spectral regime[1]. This is because the band gap and refractive index of GaN alloys can be easily controlled by changing the compositions[2]. These materials are used in laser diodes operating in visible to UV range, which can be operated at Room Temperature (RT) without cooling[3]. GaN based laser diode is fabricated using GaN/AlGaN hetero-structures, which contain GaN waveguide, embedded into $Al_x Ga_{1-x} N$ cladding layers. Under operating conditions, the temperature of the active layers of these lasers is well above room temperature, such temperature changes can influence the wave guide properties. Therefore, it is essential to know the effect of temperature on optical properties of $Al_XGa_{1-X}N$ films[4] in design of wave guides which are used in many optoelectronic applications in high power and high temperature electronics and in laser diodes[5].

This paper reports the work carried out to study the temperature dependent characteristics of GaN and AlGaN. The theoretical analysis for EBG, RI, Dielectric function[6] and model parameters has been carried out and results of simulation along with temperature drift of various parameters are presented. The paper concludes with the possible application of these results in the design of GaN waveguides, which are to be used at the elevated temperatures and for GaN/AlGaN hetero-structure lasers.

II. THEORETICAL ANALYSIS

The effective band gap of $Al_X Ga_{1-X} N$ is defined as the photon energy at which the absorption coefficient equals a value of $10^{4.8}$ cm^{-1}. The quadratic interpolation of E_g^{RT} , $E_g^{RT}(x) = 3.42+1.35\,x+0.99\,x^2$ for $0 \le x \le 6.5$ is in good agreement with the experimental data from optical transmission measurements by Spectroscopic Ellipsometry by Tisch et al.[7] The variation in EBG with respect to temperature is studied by using Bose–Einstein like expression[8,9].

$$E_g^{GaN} = E_g^{GaN}(T=0) - 2\,a_B^{GaN} / [\exp(\theta_B^{GaN}/T)-1] \quad (1)$$

Where a_B is an electron phonon coupling constant and θ_B is the average phonon temperature. The values of $E_g^{GaN}(T=0) = 3.503$ eV, $\theta_B^{GaN} = 386\pm15$ K, $a_B^{GaN} = 112\pm6$ meV are in good agreement with experimental results[9].Fig. 1 Shows the plot of effective band gap Vs temperature which shows that EBG decreases at the same rate for all compositions in the same manner over the temperature range 300K to 600K. Also Brunner et al.[4] has reported the same variation of band gap for $Al_XGa_{1-X}N$ over the whole range of composition for temperatures in the range 0 to 300K. Therefore, the composition and temperature dependant EBG, $E_g(x, T)$ can be expressed analytically as

$$E_g^{AlGaN}(x, T) = E_g^{AlGaN}(T=0) - 2\,a_B^{GaN} / [\exp(\theta_B^{GaN}/T)-1] \quad (2)$$

Let $\Delta E_g = E_g(T=0) - E_g(T=300K) = 82$ meV. It is found that ΔE_g is same for all the composition of AlGaN alloy. Therefore, EBG can be expressed in terms of $E_g^{RT}(x)$ and ΔE_g.

$$E_g^{AlGaN}(x, T) = E_g^{RT}(x) + \Delta E_g - 2\,a_B^{GaN} / [\exp(\theta_B^{GaN}/T)-1] \quad (3)$$

Where, $E_g^{RT}(x)$ is composition dependent band gap of $Al_X Ga_{1-X} N$ at room temperature.

The complex dielectric function describes the optical properties of material as a function of incident photon energy E= hυ. It is given by ε (hυ) = ε_i (hυ) = ε_r (hυ). Let us consider a linear response of AlGaN sample to a relatively weak incident radiation so that real and imaginary part of dielectric function can be connected by kramers-Kronig relations[10].The temperature dependent dielectric function of $Al_X Ga_{1-X} N$ is given by[7]

$$\varepsilon (E, x, T) = C(x, T) + [A (x, T)/ E_g(x, T)] * [(2-(1+y)^{0.5}-(1-y)^{0.5}) / y^2] \quad (4)$$

where $y = [E + i\Gamma(x, T)] / E_g (x, T)$

The shape of dielectric function is generally modified because of impurities, lattice defects and temperature broadening of transitions. The broadening factor Γ is introduced in equation 5. The photon energy E is replaced by E +iΓ. C(x, T), A(x, T) and Γ(x, T) are the temperature and composition dependent analytical model parameters used for computation of dielectric function[7]. A (x, T) is the transition strength and Γ(x, T) is the broadening factor and C(x, T) is a constant term which are given by

$$A(x, T) = [79.3 – 0.0837 T + 0.0000673 T^2 +18.99 x + 0.13T x - 0.000176 T^2 x + 37.51x^2] \text{ eV}$$
$$\Gamma(x, T) = [-8.69+ 0.0413 T + (248.24-0.19 T) x^2] 10^{-3} \text{ eV}$$
$$C(x, T) = [2.49 + 0.00227 T – 0.0000018 T^2 – 0.74 x - 0.00461T x + 0.00000533 T^2 x]$$

C, A and Γ were computed for different temperatures and compositions. The effect of temperature on them is studied.

The refractive index that is a function of incident photon energy is obtained from dielectric function,

$$n(h\upsilon, x, T) = [0.5(\varepsilon_r(h\upsilon) + (\varepsilon_r(h\upsilon)^2 + \varepsilon_i(h\upsilon)^2)^{0.5})]^{0.5} \quad (5)$$

The temperature dependence of Refractive index of GaN and AlGaN was found to be significant. The dielectric function represented by equation (4) is numerically computed and refractive index is estimated for different energies of incident photon at constant temperature of 300K and for various compositions.

III. RESULTS AND DISCUSSION

The variation in effective band gap with respect to temperature is studied for different compositions of x in $Al_XGa_{1-X}N$. Fig.1 shows the effect of temperature on EBG of $Al_XGa_{1-X}N$ for different x compositions. With increasing Al contents the EBG shifts towards higher energies for all temperatures. The EBG is almost linearly decreasing in the same proportion for all compositions with temperature.

Fig. 2 Shows the plot of dielectric function verses temperature for photon energy E=3.2 eV for various compositions. It is clear from the plot that magnitude of dielectric function increases gradually after room temperature and rate of increase is more towards higher temperature. This is due to increase in carrier concentration due to thermal excitation

The refractive index depends on energy of photon, composition and temperature. Variation in refractive index is studied for different photon energies at constant temperatures. The refractive index is found to decrease for increase in Al molar concentration at given photon energy as shown in Fig. 3. The graph reveals that for higher temperatures there is an increase in refractive index of the $Al_XGa_{1-X}N$ for a given concentration. The rate of increase of RI is almost same for all compositions up to photon energy 2.75eV and thereafter there is a drastic increase. The effects of compositional changes are much stronger than the Temperature shifts.

The model parameters C, A were found be more sensitive to change in composition than for temperature. The complex dielectric function is expressed in terms of these parameters in equation (4). The variation in these parameters with temperature is shown in Fig. 4 The transition strength A(x, T) is found to increase with increase in Al mole fraction[11,12], because the reduced mass μ of $Al_XGa_{1-X}N$ increases with increasing x. For x=0.3 to 0.5 the A(x, T) is decreasing almost linearly but for very low and high values of x we see the change in the curvature of A(x, T). C(x, T) increases with temperature for all compositions because high energy critical points are red shifted therefore their contribution to n increases. C(x, T) decreases strongly with increasing Al mole fraction this is due to high energy critical points are shifted towards higher energies and their transition strength decreases with increase in x[13]**.** Thus C(x, T) depends on x and temperature. The cause of curvature in C(x, T) is due to its dependency on x.

IV. CONCLUSION

The effect of temperature on optical properties of $Al_X Ga_{1-X} N$ alloy is studied and computer simulation is carried out within temperature range of 300-600K. Our analysis reveals that the temperature has significant effect on EBG, Refractive index and on model parameters. The decrease in effective band gap with rising temperature is in good approximation linear. The rate of decrease of EBG is same for all composition. The refractive index increases with increasing temperature for all compositions, and the changes are more prominent in the vicinity of the respective band gaps and Refractive index decreases with growing Al molar fraction. The effect of compositional changes on refractive index is much more than their corresponding temperature shifts. The Refractive index is expressed as function of Photon Energy, Temperature and composition, Refractive index of GaN and AlGaN alloys can be calculated at any desired temperature. The temperature shifts of the refractive indices of alloys should be considered

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FIGURES

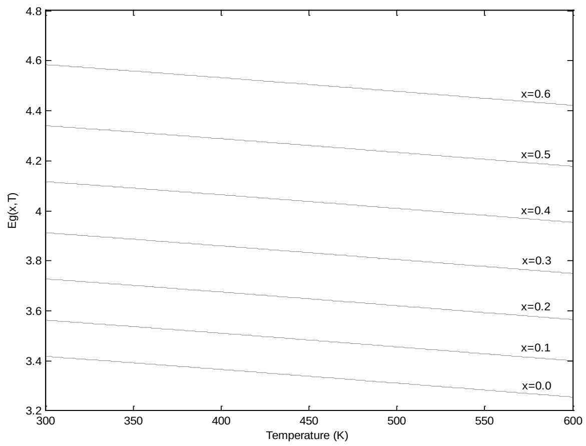

Fig. 1 Variation in Effective band gap with temperature

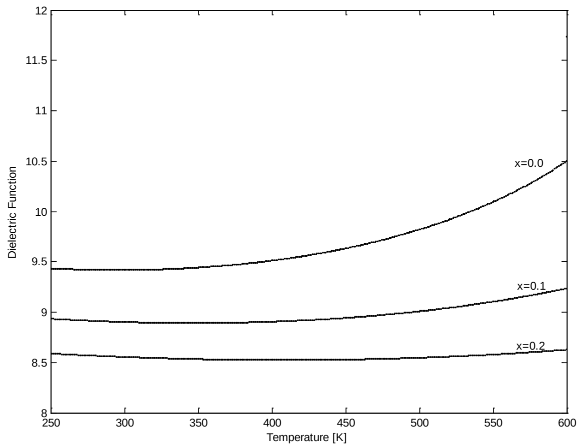

Fig.2 Variation in Dielectric Function with Temperature

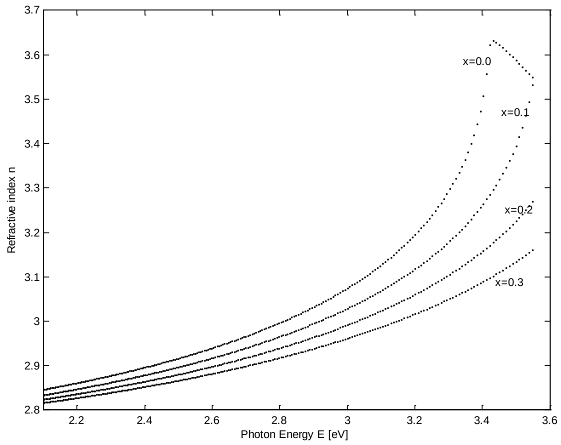

Fig. 3 Variation in Refractive Index with photon energy [eV] at 300K

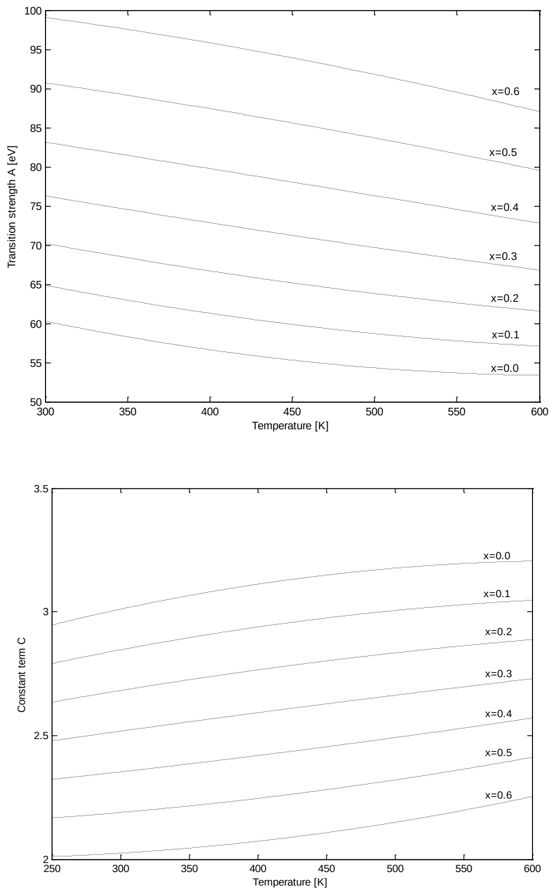

Fig. 4 Variation in Model Parameters C(x, T), A(x, T) with temperature.