Bull. Mater. Sci., Vol. 30, No. 3, June 2007, pp. 255–261. © Indian Academy of Sciences.

Theoretical analysis of effect of temperature on threshold parameters and field intensity in GaN material based heterostructure

S A GAIKWAD*, E P SAMUEL, D S PATIL and D K GAUTAM
Department of Electronics, North Maharashtra University, Jalgaon 425 001, India

MS received 13 December 2006; revised 28 February 2007

Abstract. **Temperature dependent analysis to achieve better performance by reducing threshold current requirements and field intensity has been carried out for GaN/AlGaN heterostructure lasers. The mirror loss in the GaN cavity has been obtained as a function of temperature and cavity length. The quantum efficiency has been deduced for different values of cavity length. Dependence of recombination rate on band gap and temperature has been investigated. Threshold current density has been deduced for GaN lasers and effect of temperature on it has been investigated. The near field intensity analysis has been carried out at different temperatures for 10% aluminum mole fraction in GaN/AlGaN heterostructure lasers. Furthermore, the effective index and FWHM of near field has been investigated as a function of temperature. It has been deduced from our analysis that temperature has a dominant effect on the threshold conditions and near field intensity in the wide band gap GaN based lasers.**

Keywords. **Field intensity; GaN material; heterostructure.**

1. Introduction

Recently, III–V nitride material has been of great interest in the investigation of the optical and electronic devices (Foresi and Moustakaa 1993; Craven *et al* 2004; Lin *et al* 2004). Importance of lattice dynamical properties such as phonon density and optical phonon scattering in quantum heterostructures based on group-III nitrides, GaN, AlN, InN and their ternary compounds, $Al_xGa_{1-x}N$ and $In_xGa_{1-x}N$, have been highly increased due to their potential in device applications, particularly for light emitting devices operating in blue to ultraviolet range (Chern *et al* 2003; Kim 2004; Lin *et al* 2004). Extensive studies have been carried out to enhance the performance of short wavelength lasers due to their well known applications in optical data storage and full colour display devices. Optoelectronics waveguides and light emitting devices need a sufficient refractive index step between the active layer and cladding layers for efficient confinement of light. The band gap and dielectric constant of AlGaN can be easily adapted by changing the aluminum mole fraction to provide better electrical and optical confinement, respectively, in the AlGaN/GaN heterostructure.

Radiative processes in the GaN/AlGaN heterostructures are of special importance, which usually occur in the active region of nitride-based light emitting diodes (LEDs) and laser diodes (LDs). These radiative processes are significantly influenced by temperature which affects the band gap energy and enhances the band discontinuities between GaN/AlGaN. The band discontinuities are vital for assessing the degree of carrier confinement in light emitting devices due to which the heterostructure laser diode is capable of providing optical and electrical confinement in an efficient manner. The optical confinement in the laser diode is governed by the effective refractive index of the device. The effective refractive indexes in heterostructure laser are determined through eigen value equation, which has to be solved through iterative methods.

In order to explore the full potential of GaN material for applications in heterostructure based blue–ultraviolet laser diodes, we investigated the effect of temperature on optical confinement by analysing the near field intensity. The physical parameters such as band gap energy, threshold current, mirror loss and others show great dependence on temperature (Patil and Gautam 2004). Hence, we took great care to explore the effect of temperature dependent parameters to analyse the recombination phenomena and quantum efficiency (Patil and Gautam 2002) of the heterostructure laser diode. The following section describes the mathematical approach for the investigation of temperature dependent parameters and the analysis of the recombination phenomena in the semiconductor heterostructure laser diode and results are discussed in §3.

2. Mathematical approach

Simulation tools have been developed using MATLAB software to analyse the effect of temperature on threshold

*Author for correspondence (israel_jal@sancharnet.in)

parameters and near field intensity. The refractive index, mirror loss, band gap energy, threshold current and recombination rate show the temperature dependence, while the quantum efficiency has been studied as a function of cavity length.

One of the most important optical equations to describe performance of optical devices is the wave equation. By applying proper heterointerface conditions we had optimized field solutions in different layers of the heterostructure device. Eigen value equations were used to obtain effective refractive index, N. Propagation constants in different layers of the device were computed using the following formulas:

$$\left.\begin{aligned} \gamma_c &= \sqrt{k_0^2[N^2 - n_c^2]} \quad \text{in the clad,} \\ k_x &= \sqrt{k_0^2[n_f^2 - N^2]} \quad \text{in the active layer.} \end{aligned}\right\} \tag{1}$$

$$V*\sqrt{1-b_E} = m - \tan^{-1}*\sqrt{(1-b_E / b_E + a_E)}, \tag{2}$$

where γ_c is the propagation constant in clad, k_0 the free space propagation constant at 375 nanometer wavelength, k_x the propagation constant in active region, n_c the refractive index of clad region, n_f the guiding layer refractive index, V the normalized frequency, b_E the normalized guide index, a_E the asymmetry measure of wave guide, being zero for our symmetric heterostructure, $m = 0, 1 \ldots$ is the mode value.

Field solutions have been obtained from the wave equation by using normalization conditions and heterointerface conditions along Y-direction of the device as:

$$\left.\begin{aligned} E_y &= E_{uc} * \exp(-\gamma_c y) \quad \text{in upper clad,} \\ E_y &= E_f * \cos(k_x * y + \phi_c) \quad \text{in active layer,} \\ E_y &= E_{lc} * \exp\{\gamma_c (y + d)\} \quad \text{in lower clad.} \end{aligned}\right\} \tag{3}$$

with

$$\phi_c = \tan^{-1}\left(\frac{\gamma_c}{k_x}\right),$$

where E_y represents field intensity, E_{uc}, E_f, E_{lc} are the coefficients in general solution of wave equation in upper clad, active layer and lower clad, respectively, ϕ_c the phase angle and d the active layer thickness.

The field equations are solved to analyse the laser diode structure as shown in figure 1. Thus, the above solutions are helpful to reveal the relative intensity in different layers. The structural parameters used for the analysis are listed in table 1. For the different thicknesses of the various layers, the corresponding relative intensities are observed. The refractive indices show great dependence on temperature and mole fraction variation in the GaN alloy. The refractive index of $Al_xGa_{1-x}N$ is temperature reliant and can be deduced from the following equation

$$n(E) = \left[\frac{1}{2}(\varepsilon_r(E) + \sqrt{\varepsilon_r(E)^2 + \varepsilon_i(E)^2})\right]^{1/2}, \tag{4}$$

where $\varepsilon_r(E)$ and $\varepsilon_i(E)$ are the real and imaginary parts of the dielectric function, respectively (Manasreh 1996; Tisch *et al* 2001). For active layer of GaN material we consider aluminum mole fraction, x, to be zero in $Al_xGa_{1-x}N$.

The average photon lifetime with the other absorption losses depends on the mirror loss (Patil and Gautam 2002), which has been deduced from the following formula

$$\alpha_m = (0\cdot5/l_c)*\log_e(1/(r_f*r_r)), \tag{5}$$

where l_c is the cavity length, the r_f and r_r are the front and the rear end reflectivities.

The quantum efficiency is dependent on cavity length, l_c, internal cavity losses, α_i and front end reflectivity, r_f, of the cavity. The relation of the quantum efficiency with these parameters is given below.

$$1/\eta_d = (1/\eta_{stim})(1 + (\alpha_i l_c/(\log_e(1/r_f)))). \tag{6}$$

The Shockley–van Roosbroeck formula is used for calculation of the radiative recombination rate. According to spectrum calculations and using elementary transforms, we get the following expression for spontaneous radiative recombination rate

$$R = \frac{\sqrt{\varepsilon}e^2}{m_0^2 c^3 \hbar^2} M^2 \left[\frac{2K_B T}{\Pi \hbar^2}\right] \sqrt{\mu_x \mu_y \mu_z E_g} \left[1 + \frac{3K_B T}{2E_g}\right] e^{-E_g/K_B T}, \tag{7}$$

where $\mu_x = (m_e^{-1}x + m_h^{-1}x)^{-1}$ is reduced carrier mass along x direction and similarly μ_y and μ_z for y and z, respectively

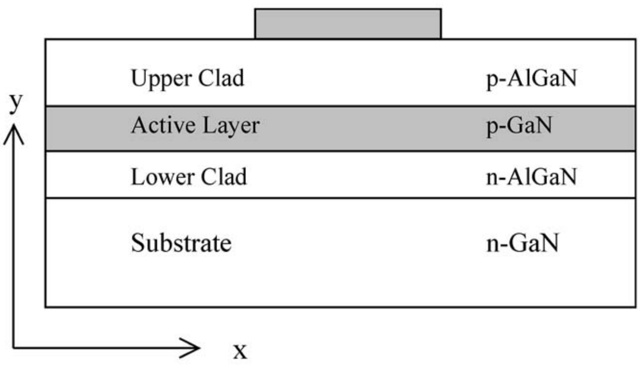


Figure 1. Typical structure of laser diode.

Table 1. Structural parameters used for the analysis.

Layer	Thickness (μm)	Aluminum (%)
Substrate	3	0
Lower clad	0·38	10
Active	0·3	0
Upper clad	0·4	10

and K_B the Boltzmann constant, M the matrix element, E_g the band gap energy of GaN, and other variables have their usual meanings.

The threshold current is the current below which there is no possibility of achieving stimulation. The following relation (Patil and Gautam 2002) can obtain this threshold current:

$$J_{\text{th}} = \frac{J_{\text{nominal}} d}{\eta_{\text{spon}}} + \frac{d}{\eta_{\text{spon}} \Gamma Q_c} \left(\alpha_i + \frac{\log_e (1/r_f)}{l_c} \right). \quad (8)$$

The investigation of the threshold current has been carried out for different values of temperature and cavity length. The analysis of the above models is realized through a graphical representation given in the following section.

3. Results and discussion

Temperature dependent analyses of refractive index, mirror loss, quantum efficiency, recombination rate, threshold current density and near field intensity have been carried out for GaN material based laser diode. The behaviour of physical parameters like band gap and recombination coefficient at higher temperature changes due to carrier overflow and smearing of quasi fermi levels, respectively. Figure 2a shows dependence of mirror loss on temperature when cavity length is 500 μm. The simulated model of mirror loss shows an increase in mirror loss in GaN cavity with respect to temperature. This is due to dependence of mirror reflectivity on the refractive index. The mirror loss shows its strong dependence on cavity length which is plotted for $T = 300$ K in figure 2b. Furthermore, with an increase in cavity length, mirror loss was observed to be decreasing drastically as shown in (5).

Figure 3 shows dependence of quantum efficiency on the cavity length. It was observed that quantum efficiency decreases nonlinearly with increase of cavity length. The stimulated efficiency was assumed to be 0·35 and internal losses in the cavity includes absorption loss, mirror loss and free carrier loss. For a fixed bias of 6 V, free carrier loss was found to be 30 cm^{-1}. Assuming thicker cladding layers in heterostructure lasers, absorption loss in substrate is assumed to be very low and its value is taken as 10 cm^{-1}. However, mirror loss is kept variable since it has strong dependence on the cavity length.

Figure 4 contains two plots combined together, the first shows variation of recombination rate with respect to

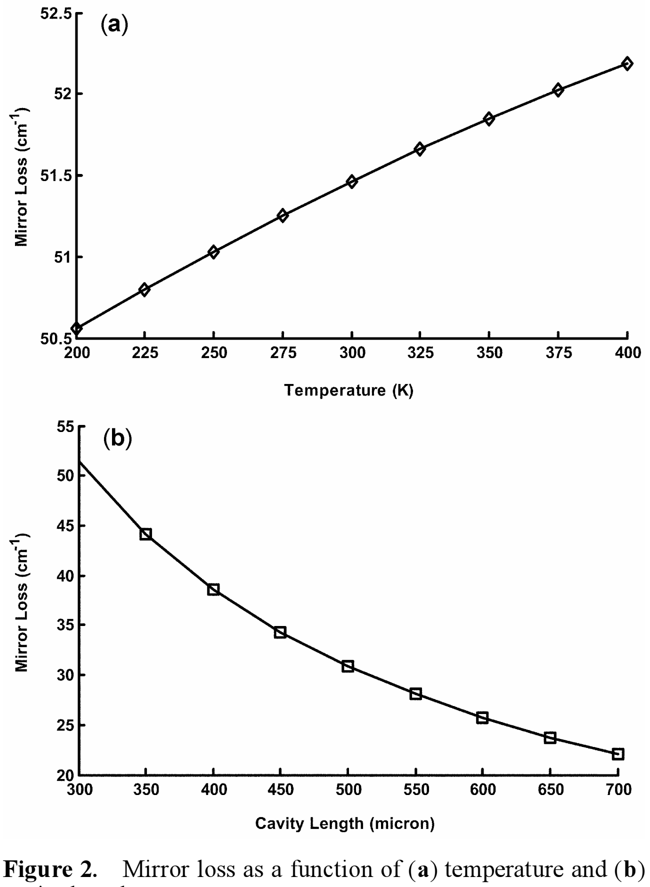


Figure 2. Mirror loss as a function of (**a**) temperature and (**b**) cavity length.

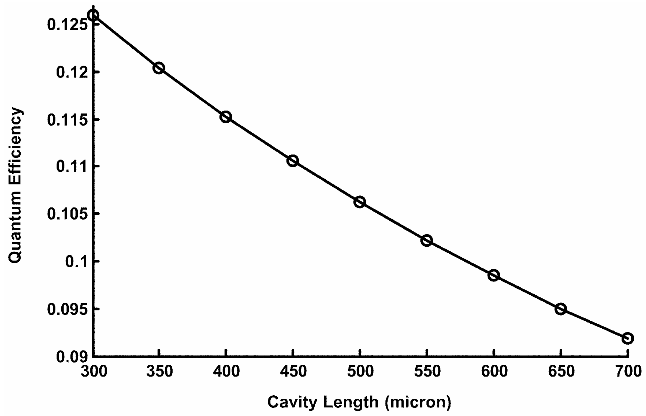


Figure 3. Dependence of quantum efficiency on cavity length.

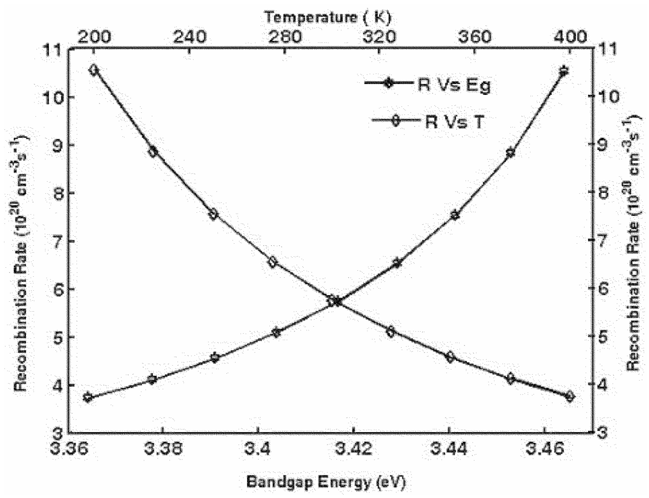


Figure 4. The variation of recombination rate with temperature and with band gap energy of GaN.

Table 2. Recombination rates at various temperatures and their corresponding band gaps for GaN material.

Temperature (K)	200	225	250	275	300	325	350	375	400
Recombination rate (10^{20} $cm^{-3}s^{-1}$)	10·548	8·8399	7·5476	6·5422	5·7417	5·0921	4·5564	4·1084	3·7293
Band gap (eV)	3·464	3·4529	3·4412	3·429	3·4165	3·4037	3·3907	3·3775	3·3641

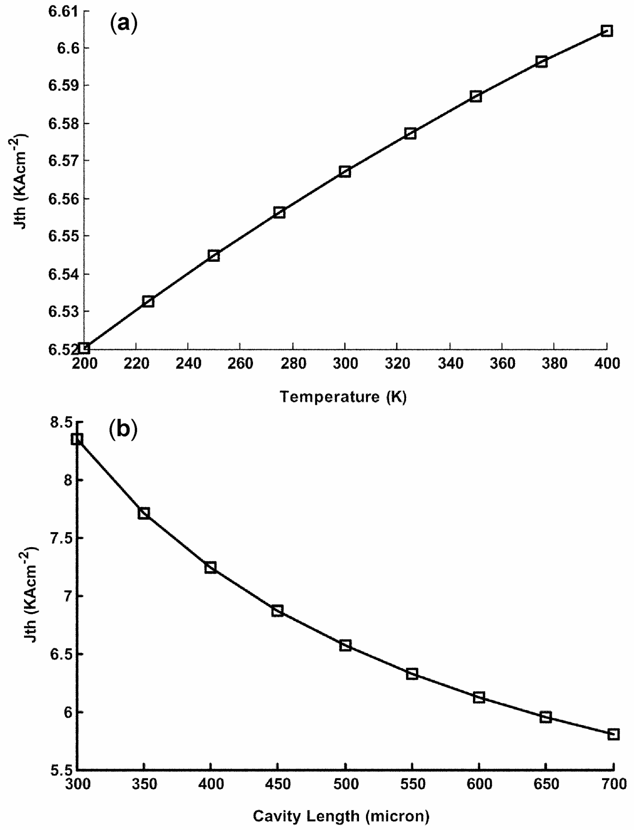


Figure 5. (**a**) Threshold current density (J_{th}) as a function of temperature and (**b**) dependence of J_{th} on cavity length.

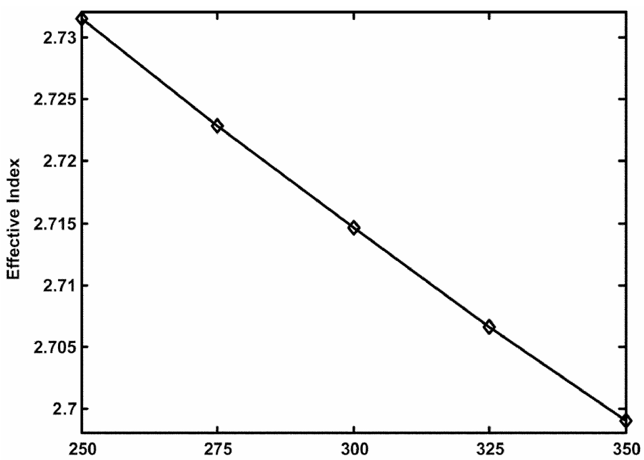


Figure 6. Effective index dependence on temperature.

temperature and the second is for recombination rate with respect to band gap energy of GaN. It is well known (Patil 2001) that spontaneous recombination rate is a function of band gap and carrier density. We have considered temperature dependence of recombination rate because in case of extrinsic semiconductor under strong injection condition values of *n* and *p* vary significantly and they depend upon intrinsic concentration which is a function of temperature. It was deduced from our analysis that recombination rate decreases nonlinearly with increase of temperature. Decrease of recombination rate with temperature is obvious due to increase in cavity losses, which further leads to increase of non-radiative recombinations in lasers. The variation of recombination rate and band gap with temperature is listed in table 2.

Figure 5a shows dependence of threshold current density (J_{th}) on temperature for the cavity length of 500 μm. It was observed from our analysis that J_{th} increases with increase in temperature. This is due to increase of cavity losses with increase of temperature, which causes more current needed to achieve population inversion to overcome cavity losses. However, J_{th} decreases with increase in cavity length due to increase of mode gain in a longer cavity laser as shown in figure 5b which is plotted for $T = 300$ K. Our results show close agreement with experimental results (Nakamura *et al* 1998).

Figure 6 shows dependence of effective refractive index on temperature. The effective index was found to be decreasing with corresponding increase in temperature. This is due to decrease of refractive indices of active and cladding regions with temperature. We had extended our analysis to near field intensity for different temperatures. The wave equation has been solved to obtain field solutions in different layers and by squaring field amplitudes; we have obtained near field intensity. The effect of temperature on field confinement is as shown in figure 7. We observed that with the increase in temperature, the field intensity spread is more at 375 nanometer wavelength due to decrease in the refractive index values of GaN and AlGaN layers. This decrease in indices values leads to decrease of effective refractive index, which consequently affects on the spread of the field. Figure 8 shows full width at half maximum (FWHM) of near field intensity as a function of temperature. It is clear that FWHM increases in a nonlinear manner with the increase of temperature. The increase in FWHM with temperature has been attributed to the spread of field intensity at higher temperatures. We have observed drastic increase in FWHM values from 0·63 μm

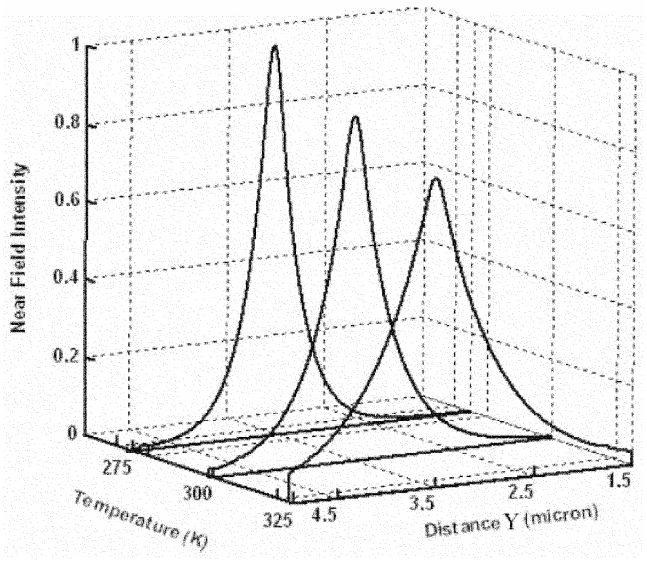


Figure 7. Near field intensity variation with distance, Y and temperature.

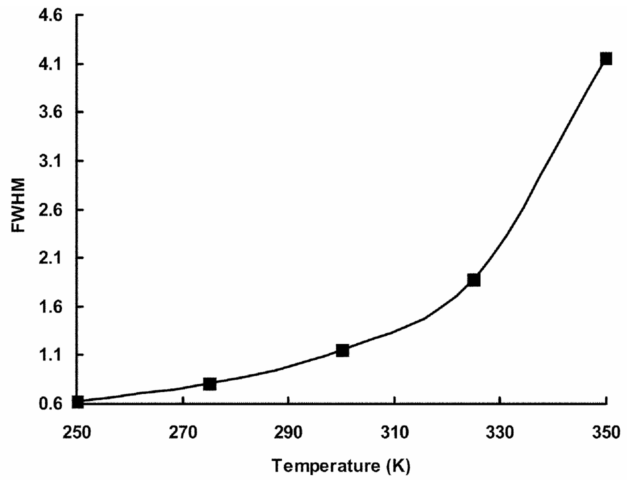


Figure 8. FWHM of near field intensity as a function of temperature.

to 4·16 μm with corresponding increase in temperature from 250 K to 350 K.

4. Conclusions

Analysis of threshold parameters and near field intensity for GaN/AlGaN heterostructure lasers has been carried out to study temperature dependent performance. We have deduced values of radiative recombination rate for GaN and studied their temperature dependence for various physical parameters of GaN based heterostructure lasers. Our study reveals that the recombination rate and energy band gap of nitride alloys have strong dependence on temperature. Our analysis is very useful to study the physical characteristics of GaN based devices at higher temperatures. It is also useful to study mirror loss in the cavity, quantum efficiency, threshold current and optical confinement.

Acknowledgements

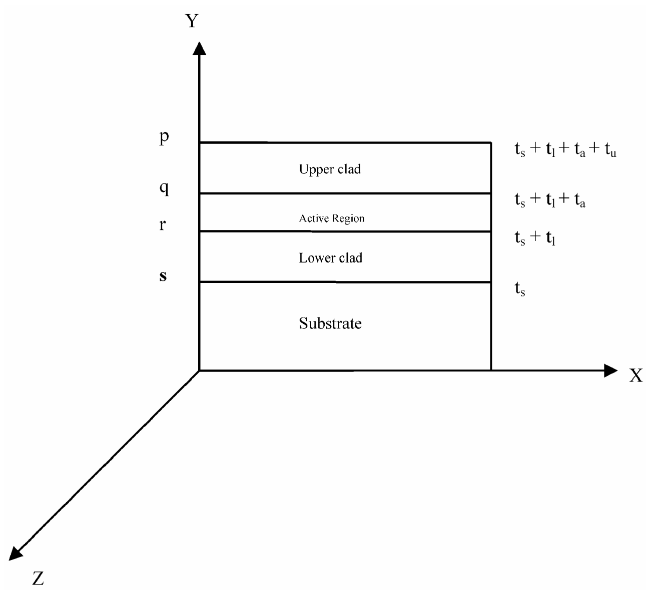
One of the authors (SAG) is thankful to the University Grants Commission, for providing a Teacher fellowship and JDMVP Samaj Ltd., Jalgaon, for study leave for carrying out this work. One of the authors (DSP) gratefully acknowledges the financial support through a Young Scientist Project from the Department of Science and Technology, New Delhi.

Appendix A

The semiconductor laser diode operation involves an interaction of optical and electrical equations. The wave equations obtained from differential form of Maxwell's equations are used to describe optical field distribution in the laser diode,

$$\nabla^2 E(x, y) + (k_0^2 n^2 - \beta^2)E = 0,$$

where β is the mode propagation constant, k is called propagation constant and n the refractive index. The wave equation is solved using effective index method. Effective index is determined using eigen value formula for three-layer wave guide structure assuming negligible absorption loss in the substrate. The following figure shows the typical laser diode structure used to find out the optical field intensity in various layers. t_s, t_l, t_a, t_u are the thicknesses of substrate, lower clad, active region and upper clad, respectively and points p, q, r, s represent the limits of integration along Y direction in various layers.



The waveguide theory is applied to semiconductor laser diode structure to compute optical field components. The active region of the semiconductor laser acts as a light guiding layer and is sand-wiched between covering layers of clad region. The solution for wave equation is obtained for transverse electric mode only by assuming that light generated is fully polarized. The general solutions of transverse electric field in different layers are assumed as,

$$E_u = E_c \exp[-\gamma_c (y - p)] \quad \text{where } y \text{ is in upper clad,} \quad (1)$$

$$E_a = E_f \cos\{[k_x (y - q)] + \phi_c\} \quad \text{where } y \text{ is in active region,} \quad (2)$$

$$E_l = E_s \exp[\gamma_s (y - r)] \quad \text{where } y \text{ is in lower clad.} \quad (3)$$

By applying boundary conditions at the interface of the layers, we determine the coefficients, E_s, E_c and E_f in the above solution and compute field intensity variation with respect to distance, y, in various layers of laser diode.

At the interface of lower clad and active region, i.e. at $y = r$, $E_l = E_a$, then from (2) and (3) we get,

$$E_f \cos\{[k_x (r - q)] + \phi_c\} = E_s. \quad (4)$$

At the interface of upper clad and active region, i.e. at $y = q$, $E_u = E_a$, then from (1) and (2) we get,

$$E_c \exp[-\gamma_c (q - p)] = E_f \cos\phi_c, \quad (5)$$

where ϕ_c is the phase angle given by $\phi_c = \tan^{-1}(\gamma_c / k_x)$.

Using normalization method,

$$\int_s^r E_s^2 \exp\{2[\gamma_s (y - r)]\} dy + \int_r^q E_f^2 \cos^2\{[k_x (y - q)] + \phi_c\} dy + \int_q^p E_c^2 \exp\{2[-\gamma_c (y - p)]\} dy = 1.$$

Solving the integration we get,

$$E_s^2 \left[\frac{\exp 2[\gamma_s (y - r)]}{2\gamma_s}\right]_s^r + E_f^2 \int_r^q \frac{1 + \cos 2\phi_c}{2} dx + E_c^2 \left[\frac{\exp 2\{-\gamma_c (y - p)\}}{-2\gamma_c}\right]_q^p = 1,$$

$$E_s^2 \left[\frac{1}{2\gamma_s} - \frac{\exp 2[\gamma_s (t_s + t_r)]}{2\gamma_s}\right] + E_f^2 \left[\frac{y}{2}\right]_r^q + \left[\frac{\sin 2\phi_c}{4k_x}\right]_r^q + E_c^2 \left[\frac{1}{-2\gamma_c} + \frac{\exp 2[-\gamma_c (q - p)]}{2\gamma_c}\right] = 1,$$

$$E_s^2 \left[\frac{1 - \exp 2[\gamma_s (-t_l)]}{2\gamma_s}\right] + E_f^2 \left[\frac{t_a}{2} + \left(\frac{\sin 2\phi_c}{4k_x}\right) - \frac{\sin 2[k_x (-t_a) + \phi_c]}{4k_x}\right] + E_c^2 \left[\frac{\exp 2(\gamma_c t_u) - 1}{2\gamma_c}\right] = 1,$$

$$E_s^2 \left[\frac{1 - \exp 2[\gamma_s (-t_l)]}{2\gamma_s}\right] + E_f^2 \left[\frac{t_a}{2} + \frac{\sin 2[k_x t_a - \phi_c] + \sin 2\phi_c}{4k_x}\right] + E_c^2 \left[\frac{\exp 2(\gamma_c t_u) - 1}{2\gamma_c}\right] = 1. \quad (6)$$

Let

$$\left[\frac{1 - \exp 2[\gamma_s (-t_l)]}{2\gamma_s}\right] = U,$$

$$\left[\frac{t_a}{2} + \frac{\sin 2[k_x t_a - \phi_c] + \sin 2\phi_c}{4k_x}\right] = M,$$

$$\left[\frac{\exp 2(\gamma_c t_u) - 1}{2\gamma_c}\right] = L,$$

substituting in (6) we get,

$$E_s^2 U + E_f^2 M + E_c^2 L = 1. \quad (7)$$

Using (4) and (5), E_s and E_c can be expressed in terms of E_f

$$E_s = E_f \cos(k_x t_a - \phi_c), \quad (8)$$

$$E_c = \frac{E_f \cos\phi_c}{\exp[-\gamma_c (-t_u)]} = \frac{E_f \cos\phi_c}{\exp[\gamma_c t_u]}. \quad (9)$$

Let, $\cos(k_x t_a - \phi_c) = A$,

$$\frac{\cos\phi_c}{\exp[\gamma_c t_u]} = B,$$

$$E_s^2 = E_f^2 A^2,$$

$$E_c^2 = E_f^2 B^2.$$

Substituting in (7), we evaluate E_f as follows

$$E_f^2 A^2 U + E_f^2 M + E_f^2 B^2 L = 1,$$

$$E_f^2 [A^2 U + M + B^2 L] = 1.$$

Thus, after computing E_f, using the above relation, the components, E_s and E_c, are determined numerically using (8) and (9). This way we compute the optical field intensity in various layers of GaN/AlGaN heterostructure laser.

Appendix B

N, effective refractive index; k_0, free space propagation constant; k_x, propagation constant in active region; γ_c, propagation constant in clad region; n_c, refractive index of clad region; n_f, guiding layer refractive index; V, normalized frequency; b_E, normalized guide index; a_E, asymmetry measure of wave guide; m, mode number value; E_y, field intensity in various layers; E_{uc}, coefficient in general solution in upper clad; E_f, coefficient in general solution in active region; E_{lc}, coefficient in general solution in lower clad; ϕ_c, phase angle; x, mole fraction; $n(E)$, refractive index as a function of photon energy; $\varepsilon_r(E)$, real part of dielectric function; $\varepsilon_i(E)$, imaginary part of dielectric function; α_m, mirror loss; α_i, internal cavity losses; l_c, cavity length; r_f, front end reflectivity; r_r, rear end reflectivity; η_d, quantum efficiency; η_{stim}, stimulated efficiency; η_{spon}, spontaneous efficiency; R, recombination rate; μ_x, reduced carrier mass along x direction; K_B, Boltzmann constant; E_g, band gap energy; m_0, electron mass; c, speed of light; e, electronic charge; M, matrix element; T, temperature; ε, dielectric constant; J_{th}, threshold current density; $J_{nominal}$, nominal current density; Q_c, gain constant; d, active layer thickness; Γ, confinement factor.

References

Chern G D *et al* 2003 *Appl. Phys. Lett.* **83** 1710

Craven M D *et al* 2004 *Appl. Phys. Lett.* **84** 496

Foresi J S and Moustakaa T D 1993 *Appl. Phys. Lett.* **62** 2859

Kim Joo Han 2004 *Appl. Phys. Lett.* **84** 711

Lin Kung-Hsuan *et al* 2004 *Phys. Rev.* **B70** 073307-1

Manasreh M O 1996 *Phys. Rev.* **B53** 16425

Nakamura Shuji *et al* 1998 *Appl. Phys. Lett.* **72** 2014

Patil D S 2001 *Design, analysis and fabrication techniques of blue laser diode*, Ph D Thesis, N M University, Jalgaon

Patil D S and Gautam D K 2002 *Opt. Commun.* **201** 413

Patil D S and Gautam D K 2004 *Physica* **B344** 140

Tisch U *et al* 2001 *J. Appl. Phys.* **89** 2676