Temperature dependent analysis of refractive index, band gap and recombination coefficient in nitride semiconductor lasers

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Received 5 June 2006; revised 3 January 2007; accepted 22 January 2007

Temperature dependent analysis of recombination coefficient, band gap and refractive index has been carried out to explore applicability of nitride lasers at higher temperatures. To estimate recombination coefficient at various temperatures Shockley-van Roosbroeck model has been used. Our results reveal that refractive index increases in linear manner with temperature and indium mole fraction in InGaN. However, refractive index was found to be decreasing with Al mole fraction and temperature in non-linear manner. The band gap deduced from our analysis was found to be increasing with Al mole fraction and decreasing with In mole fraction and therefore, these alloys provide better opportunity to form effective heterostructures with GaN. The recombination coefficient analysed, was observed to be decreasing non-linearly with band gap and temperature for AlGaN. However, in case of InGaN, the recombination coefficient shows linear increase with band gap and non-linear decrease with temperature.

Keywords: Recombination coefficient, Band gap, Refractive index, Nitrides, Semiconductor lasers
IPC Code: H01S 5/00

1 Introduction

Now-a-days, III-V compound semiconductors provide the materials basis for a number of well-established commercial technologies, as well as in short wavelength lasers. Some of the examples include high-electron-mobility and heterostructures bipolar transistors, diode lasers, light-emitting diodes, photo-detectors, electro-optic modulators, and frequency-mixing components. The operating characteristics of these devices depend on the physical properties of the constituent materials. AlGaN and InGaN alloys are attracting much attention as candidate materials for realizing deep ultraviolet (UV), light-emitting diodes or laser diodes. The short wavelength lasers using these compounds have been realized as efficient light sources. Semiconductor light sources operating in the UV region are required for a number of applications, including long lifetime white lighting, sterilization and decontamination, for use in the medical field and biochemical processes, for the purification of the environment, and for high-density optical storage. Despite of these, they are very important for household air cleaners, automobile exhaust purifiers, UV sensing systems and so on.

Although, light sources using gallium nitride based compounds have been realized successfully, there is a lot of scope remains to improve the efficiency of these devices by studying their physical mechanism on the basis of material properties to enhance their performance and characteristics. The computer analysis helps in determining the critical physical parameters and their temperature dependence for applicability in power applications. The analysis of effect of temperature on ZnSSe based blue laser diode characteristics at 507 nm wavelength has been reported.

The performance of the device is greatly affected at higher temperatures due to carrier overflow, which insist for greater value of band gap discontinuity. The stringent requirement for the stimulated emission in the laser diodes is greater probability of radiative recombination. The rate of recombination has strong dependence on band gap of material, which consequently depends on the temperature. Optical confinement is mainly controlled due to refractive index step between active region and cladding layers. High temperature operation demands changing values of refractive indices, which further changes the possibility of the optical confinement.

The main objective of this work is to analyze temperature dependence of refractive index, band gap and recombination coefficient, which affects radiative recombination and optical confinement in nitride semiconductor lasers. We have carried out the
detailed analysis using MATLAB to investigate the effect of temperature on ternary alloys of GaN, namely AlGaN and InGaN. Our analysis helps in improving the performance of the light emitting devices based on GaN at higher temperatures. The models of recombination coefficient, band gap and refractive index have been studied and simulated using MATLAB.

2 Models of Physical Parameters for AlGaN and InGaN

2.1 Modeling of recombination coefficient

Shockley-van Roosbroeck formula is used for calculation of the radiative recombination intensity, to calculate transition rate. Total spontaneous emission rate has been obtained by taking integration over all energy values to include states in the conduction and valance band relevant to luminescent process:

\[ R_s = \int r_s(E) dE \quad \ldots (1) \]

where \( r_s \) is spectral function of spontaneous recombination.

From quantum mechanical calculations, the spectral density of transition probability with emission of photon with energy \( E_k \) and arbitrary polarization and arbitrary direction of wave vector \( k \).

\[ W_{cv} = \frac{2e^2 \sqrt{\varepsilon \eta \omega}}{m_0^2 v_c^3 \eta^2} M^2 [N(E_k) + 1] d(E_c - E_v - E_k) \]

where \( \sqrt{\varepsilon} \) = Refractive index
\( m_0 \) =Free electron mass

\[ M^2 = \frac{1}{4\pi} \sum_{A=1} \int d\Omega_k |e_{kA} P_{cA}|^2 \quad \ldots (3) \]

where \( M \) is the Matrix element. \( e_{kA} \) is polarization vector of photon with momentum \( k \), \( P_{cA} \) is interband transition matrix element, \( E_c \) and \( E_v \) electron and hole energy, respectively.

Using Fermi Dirac function for non-degenerate semiconductor and summing it with one of the wave vector \( (kv) \) we obtain:

\[ r(s)(\eta \omega) = \int \eta \omega d(\eta \omega) e^{E_v - E_c + \frac{1}{2}k^2 T} \]

\[ d\left[ E_{c(k)} - E_v(k) - \eta \omega \right] d^3k \quad \ldots (4) \]

According to spectrum calculation and using elementary transform, we get the following expression for spontaneous radiative recombination rate.

\[ R = \frac{\sqrt{\varepsilon \eta \omega}}{m_0^2 v_c^3 \eta^2} M \left[ \frac{2k_bT}{\Pi \eta} \right] \sqrt{\mu_x \mu_y \mu_z} E_g \]

\[ \left[ 1 + \frac{3k_bT}{2E_g} \right] e^{-E_g/k_bT} \quad \ldots (5) \]

where \( \mu_e = (m_e^{-1}x + m_h^{-1}x)^{-1} \) is reduced carrier mass direction and similarly for \( y \) and \( z \).

Defining radiative recombination rate as:

\[ R = Bnp \quad \ldots (6) \]

where \( n \) and \( p \) are carrier concentration and using well-known expression for concentration of electron and holes in non-degenerate semiconductor.

\[ np = (4m_e m_h)^{1/2} \frac{k_b T}{2\pi \eta^2} \exp\left( \frac{-E_g}{k_b T} \right) \quad \ldots (7) \]

We get the expression like:

\[ B = \frac{\sqrt{\varepsilon \eta \omega}}{m_0^2 v_c^3 \eta^2} M \left[ \frac{2\Pi \eta^3}{k_b T} \right]^{3/2} \left( \frac{1}{m_e m_h m_i} \right)^{3/2} \quad \ldots (8) \]

\[ E_{gs}(T) \left[ 1 + \frac{3k_b T}{2E_g(T)} \right] \]

where \( B \) is radiative recombination coefficient, which depends on the temperature, carrier density and band structure of the semiconductor material. The expression for \( B \) has been obtained from band to band transition model with \( M \) as the matrix element as
defined by Eq. (3). All the calculations have been carried out at the Γ point of the band where, value of \( k \) is zero. Value of \( M \) has been obtained by taking summation of the integral of momentum transition element over the momentum space. We have used Simpson’s numerical integration method to obtain value of \( M \). The value of temperature dependent band gap for the ternary compounds of GaN have been obtained using Varshni formula as specified in Eq. (9).

2.2 Modeling of band gap

Vegard’s law describes the linear interpolation of band gap as a function of alloy composition. In case of AlGaN alloys, the approximation is reasonably accurate but there is substantial non-linearity in band bowing is observed.

The temperature dependence of band gap of semiconductors is given by Varshni formula:

\[
E_g(T) = E_g(0) - \frac{\gamma T^2}{T + \beta} \quad \ldots (9)
\]

where \( \gamma \) and \( \beta \) are parameter. Their values for GaN, AlN nitrides are given in Refs (16 and 17). We have computed the band gap of GaN and AlN at various temperatures and for evaluating band gap in the binary alloys of the components A and B, we used following expression where \( d \) is the bowing parameter.

\[
E_g^{(AB)}(x, T) = [xE_g^{(A)}(T) + (1 - x)E_g^{(B)}(T)] - dx(1 - x) \quad \ldots (10)
\]

The band gap of AlGaN and InGaN depend upon the Al or In mole concentration \( x \) and temperature. The band gaps of AlGaN and InGaN at various temperatures for varying values of molar concentration have been evaluated. For each value of molar concentration, we have got a set of values of band gaps of AlGaN and InGaN for corresponding temperatures. These sets of values are used to compute the radiative recombination coefficient at various temperature for AlGaN and InGaN materials.

2.3 Modeling of refractive index

The refractive indices show great dependence on temperature and mole fraction variation in the GaN alloy. The refractive index of Al\(_x\)Ga\(_{1-x}\)N decreases with the increase of temperature and aluminium mole fraction. The refractive indices have been deduced from the following equation:

\[
n(E) = \frac{1}{2} \left( \varepsilon_r(E) + \sqrt{\varepsilon_r(E)^2 + \varepsilon_i(E)^2} \right)^{\frac{1}{2}} \quad \ldots (11)
\]

where, \( \varepsilon_r(E) \) and \( \varepsilon_i(E) \) are the real and imaginary part of dielectric function, respectively.

3 Results and Discussion

Temperature dependent analysis of refractive index, band gap and recombination coefficient have been carried out for AlGaN and InGaN alloys to explore the applicability of GaN based compounds for high power devices at higher temperatures. 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. The simulated model of refractive index shows linear increase over In mole fraction and temperature as shown in Fig. 1. The refractive index value was found to be changing from 2.5 to 3.4, respectively with increase of mole fraction from 0 to 100%. This provides very good waveguide mechanism property between InGaN and GaN. However, refractive index shows little change with respect to temperature from 2.78 to 2.793 with corresponding change in temperatures from 200 to 400 K. The variation of refractive index of AlGaN with Al mole fraction and temperature is shown in Fig. 2. The refractive index was found to be decreasing from 2.35 to 1.97 with Al mole fraction of 0 to 100%, respectively. Therefore, AlGaN can be
used as cladding layer to form perfect waveguide with GaN for higher values of Al mole fraction and provides better optical confinement. However, temperature dependent analysis shows very little change in refractive index for AlGaN.

Fig. 3 shows the variation of band gap energy with Al and In mole fractions in AlGaN and InGaN alloys, respectively. The band gap of these alloys can be easily tailored by adding either Al or In. This provides sufficient band gap discontinuity to have electrical confinement of carriers in nitride heterostructures. Increase of Al mole fraction increases the band gap in non-linear manner while band gap decreases with increase of In mole fraction. Our simulated results show band gap tailoring from 3.3 to 5.8 eV for AlGaN and from 3.4 to 1.98 eV with increase of mole fraction from 0 to 100%.

The recombination in the semiconductors is the physical phenomenon, which could be radiative or non-radiative. In the radiative recombination process, energy produced is emitted as a light in the form of photons to the outside of the semiconductors. The radiative recombination processes are most useful for the efficient light emission from the semiconductor devices. The spontaneous emission recombination rate is directly proportional to the product of carrier densities with proportionality constant as recombination coefficient $B$. It has strong dependence on carrier density, band gap and temperature. Our analysis shows dependence of $B$ on band gap and temperature for both the alloys as illustrated in Figs 4 and 5. The recombination coefficient from our
analysis was found to be decreasing from $2.7 \times 10^{-11}$ to $1.45 \times 10^{-11}$ cm$^3$/s for AlGaN at 300 K temperature with increase of band gap energy. However, for the 30% Al mole fraction, value of $B$ decreases from $3.78 \times 10^{-11}$ to $1.45 \times 10^{-11}$ cm$^{-3}$/s with corresponding increase in temperature from 200 to 350 K. The decrease in $B$ has been attributed to increase of non-radiative recombinations at higher temperatures. The recombination coefficient from our analysis was deduced to be increasing with respect to band gap from $2.1 \times 10^{-11}$ to $3 \times 10^{-11}$ cm$^3$/s for InGaN at 300 K temperature. However, for the 30% In mole fraction value of $B$ decreases from $4.07 \times 10^{-11}$ to $1.45 \times 10^{-11}$ cm$^{-3}$/s with corresponding increase in temperature from 200 to 350 K.

4 Conclusion

We have extracted values of radiative recombination coefficient for GaN and their ternary alloys and studied their temperature dependence for various doping concentrations. This recombination coefficient is very important in laser diode modeling as it decides the intensity of emission of radiation. The recombination coefficient decreases with increase of temperature due to increase of non-radiative recombinations and decrease of radiative recombinations. For wide band gap materials, value of $B$ is greater according to band-to-band transition model$^{19}$. Our analysis shows that value of $B$ is increasing with increasing of band gap, as expected. Our study reveals that the recombination coefficient and energy band gap of nitride alloys have strong dependence on temperature and weak dependence on refractive indices of these alloys. Our results show excellent agreement with experimental and theoretical results reported by researchers$^{20}$. Our analysis is very useful to study the physical characteristics of GaN based devices at higher temperatures and their degradation in performance with increase in temperature.

Acknowledgement

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

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