Carrier transport studies and scattering mechanism in GaN/AlGaN superlattice for high speed lasers

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Optimization of physical parameters of GaN/AlGaN superlattice structure has been carried out to ensure both fast carrier transport and efficient capture into quantum confined states through scattering mechanism for the development of high speed lasers. The interaction of electrons with the optical phonons has been considered for the scattering of electrons by emission of optical phonons for studying physical properties of superlattice. The electron confinement in a superlattice structure has been realized for odd and even number of quantum wells. Transfer Matrix Method (TMM) had been used to obtain the wave function intensity. The effect of material composition on barrier height and energy has been explored and the effect of eigenenergy variation on the transmission coefficient and Scattering rate has been investigated. The better electron confinement has been obtained at the center of the superlattice structure as expected. It reveals from our analysis that the scattering rate decreases with increase in aluminum mole fraction and increases linearly with the increase in temperature considerably. Scattering rate was found to increase linearly with the increase in wavelength and it has been attributed to the increase in eigenenergy and static dielectric constant.

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1. Introduction

The III-V nitrides and their alloys are promising materials for light emitting devices [1-4] operating in the visible and ultraviolet range. Due to wide direct band gap and strong inter-atomic bonds they are suitable semiconductor materials [5-8] for the realization of high temperature and high power devices. A variety of device structures have been fabricated using GaN. These include double heterostructures, single quantum wells, multiple quantum wells and superlattice structures. Band gap engineering of semiconductor quantum well (QW) heterostructures provides the possibility of controlling the electronic and optical properties of quantum well lasers by varying the parameters like layer thickness and material compositions.

Furthermore, the complex quantum structures like multiple quantum well and super lattice provide large optical gain, low threshold current density and better confinement. Therefore, it is required to analyze the quantum wells of Gallium Nitride sandwich between the AlGaN barriers, which provides an excellent electron confinement [9]. Multiple quantum well and superlattice structure shows a great variation in electrical properties due to their different structural parameters.

The electron motion is quantized in quantum structures when the de Broglie wavelength is comparable to the dimension of the region in which the electrons are confined. In GaN/AlGaN structures, the electron confinement is supported by the energy band edge discontinuities at the interfaces between different materials. The coupling between electronic states localized in superlattice structures is of great importance for the device technology. When the attenuation length of the electronic wave function into the barriers becomes comparable with the barrier thickness, the carrier tunneling between adjacent wells modifies the transport properties and recombination mechanism forming the minibands in periodic structures.

For studying the optical and electrical properties in GaN/AlGaN superlattice structures, the intra sub band and inter sub band scattering rates for electrons and holes by emission of optical phonons is of prime importance. The interaction of electrons with optical phonons leads to significant changes in the operational behavior of such structures. These interactions control the energy and momentum relaxation processes, which affect the performance and speed of the device. Fermi golden rule describes the scattering probability of the carrier scattering [10-11] from the energy sub band above the quantum well to the energy sub band in the quantum well.

This paper concerns with study of carrier transport in GaN/AlGaN superlattice structure. The optimization of physical parameters of superlattice structure has been carried out through quasi-transmitting boundary method (QTBM) applied to Schrödinger equation. The electron confinement in a superlattice structure has been realized for odd and even number of quantum wells. To obtain the wave function intensity we had used Transfer Matrix Method (TMM) [12] the efficient and more accurate method, to determine the eigenenergy. The effect of Eigen energy variation on the transmission coefficient and Scattering rate has been investigated. Furthermore, scattering rate dependence on temperature and wavelength has been studied for the different values of aluminum material composition.

The following section explains a detail mathematical analysis to study carrier transport for the electron confinement and scattering rate investigation. Finally, results have been discussed properly with their physical significance and importance.

2. Mathematical analysis

In order to get theoretical insight in superlattice, we apply a simplified theoretical approach of the electron confinement and electron-phonon scattering rate. The energy levels and wave functions of the superlattice were obtained by numerical solution of the effective mass Schrödinger equation [13]. It is essential to optimize electrical and physical parameters to fabricate the III-V nitride based semiconductor superlattice structure. The properties like effective mass, barrier height are generally accepted for the calculation of energy levels within the quantum wells. The variation of effective mass and band offset on energy is very important. Ψ(x), the time independent Schrödinger equation is the wave function that describes the spatial behavior and E is the energy of electron. The standard Schrödinger equation can be written as given in equation (1). In the well region, conduction band potential V is assumed to be zero and m* is effective mass of Gallium Nitride, where as in the barrier region conduction band potential is V and m* is effective mass of $Al_xGa_{1-x}N$. For confinement of the electrons in the well region, the energy E must be less than the barrier height V.

$$\partial^2\psi(x)/\partial x^2 = (8\, m^*\, \pi^2/h^2)\,(V - E)\,\psi(x) \qquad (1)$$

For solving the wave function two important boundary conditions are used. The first boundary condition is that Ψ must be continuous and second is that ∂Ψ /∂x must be continuous. Further, the normalization condition has to be used for determination of the arbitrary constants. The general solutions Ψ(x) of the Schrödinger equation for the barrier region and quantum well region in a superlattice structure (SLS) for i number of layers are given as follows

$$\left.\begin{aligned}\psi_b(x) &= A_{bi}\exp(qx) + B_{bi}\exp(-qx),\\ \psi_w(x) &= A_{wi}\sin(kx) + B_{wi}\cos(kx),\end{aligned}\right\} \qquad (2)$$

At this juncture, $\psi_b(x)$ and $\psi_w(x)$ are the general solutions of barrier and well region respectively, A and B are arbitrary constants, the suffixes b, w, and i are barrier, well and the number of layer respectively. The q and k are the wave vectors of the barrier region and well region respectively. The wave vectors can be obtained from the following expressions:

$$k = \frac{\sqrt{2m^*E}}{\hbar}, \quad \text{and} \quad q = \frac{\sqrt{2m^*(V - E)}}{\hbar} \qquad (3)$$

These wave vectors are determined by obtaining first the transcendental equation using the transfer matrix method and thereafter through an iterative method (secant method) the transcendental equation has been solved to calculate Eigen energy. In transfer matrix method, all the matrices are combined in such a way that the coefficient of outer regions are linked. The matrices, which are use for the solution of Eigen energy, are useful for calculating the transmission coefficients. The reduced product of these matrices is 2 × 2 matrix, which is given by the following equation (4),

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = M \begin{pmatrix} A_n \\ B_n \end{pmatrix} \qquad (4)$$

Here, M is product of all the matrices obtained through the coefficients of arbitrary constants of the general solutions of the Schrödinger equation in each layer of the superlattice structure by applying boundary conditions as mentioned earlier. The suffix n denotes the top most layer of the superlattice structure. Then one can obtained the arbitrary constant by converting the 2 × 2 matrix in the form of expressions as follows.

$$\begin{aligned} A_1 &= M_{11}A_n + M_{12}B_n \\ B_1 &= M_{21}A_n + M_{22}B_n \end{aligned} \qquad (5)$$

The probability interpretation of the wave function implies that the wave function must tend towards zero into the outer barriers, i.e. the coefficients of the growing exponentials must be zero. Therefore, at the first and last interface, B_1=0 and A_n =0, and hence in the above equation we gets M_{22} = 0, since B_7 cannot be zero. As all of the elements of M are function of the k and q, which are again the function of the energy E, they have to satisfy the condition that $M_{22}(E) = 0$. This approach and variations upon it are often referred to as the *transfer matrix technique*. Once the energy is known, the coefficients A_1 to B_n follow simply and the envelope wave function can be deduced and the transmission coefficient is given by the following expression:

$$T(E) = \frac{1}{M^*_{11}M_{11}} \qquad (6)$$

Here M^*_{11}, describes the conjugate form of matrix

The first element of the above equation is employed to determine the transmission coefficient. The motive behind using the transfer matrix method was to obtain the electron energy accurately and to analyze the transmission coefficients concurrently. The transmission coefficient is necessary to study the tunneling of the electron from the quantum well regions. The transmission coefficient has been an important quantity since it provides most of the relevant information of the transport process in SLS, and is characterized by a series of resonance peaks at specific energies. The properties of these transmission resonances and their implications on the electronic transport in semiconductor heterostructures have been extensively studied using solutions of the time-independent Schrödinger equation [14].

The optical phonons have significance for studying the electrical and optical properties in a complex quantum structures. The interactions of electrons with the optical phonons in multiple quantum wells and superlattice structure are of crucial importance in the physics of semiconductor heterostructures. The carrier scattering have received special theoretical attention because of quantum mechanical aspects, which plays an important role in a carrier transport phenomena. There are a number of models used for the description of optical phonons in a layered system though the bulk phonon models, which are still applicable. In this paper, we explored using well-known Fermi Golden Rule, the scattering rates of electrons in bulk bands with longitudinal optic phonons in superlattice structure. Here we considered the scattering rate as a function of temperature, wavelength and aluminum concentration.

The scattering rates of electrons in bands with these longitudinal optic phonons, involves many of the mathematical techniques required for the analysis of quantization effect in complex quantum structures such as superlattice. The electron-optical phonon scattering limits the electron mobility and hence drastically affects the electron hole recombination process in a superlattice structure. Hence, the electron-phonon interaction in superlattice structure has been taken into account in Fermi Golden Rule equation for the realization of scattering rate of electron. The following expression of electron-phonon interaction (H) includes the crystal volume (V) and momentum of phonon (K).

$$\mathrm{H} = e\sum_{K}\left(\frac{\hbar\omega p}{2|K|^2}\right)^{\frac{1}{2}}\frac{e^{-iK.x}}{V^{\frac{1}{2}}} \tag{7}$$

$$\frac{1}{\tau_i} = \frac{2\pi}{\hbar}\sum_{f}\left|\langle f|\mathrm{H}|i\rangle\right|\delta(E_f - E_i) \tag{8}$$

The scattering rate has been deduced using the Fermi Golden Rule equation, which provides accurate evaluation of transition probability [15] from the initial (E_i) and the final (E_f) energy state. Replacing H in equation (8) from equation (7) and by converting the sum over phonon momentum to integral the scattering rate turns to

$$\frac{1}{\tau_i} = \gamma'\int_0^{\pi}\int_0^{\infty}\delta\left(K^2 + 2Kk_i\cos\Phi + \frac{2m^*\omega}{\hbar}\right)dK\,\sin\Phi\, d\Phi \tag{9}$$

Where, Φ is the angle, which determines initial and final states of phonon momentum and ω is the phonon frequency. Since, the integration is over phonon momentum, this argument can be factorize in the following manner, considering the angle ϕ between the initial (k_i) and final (k_f) momentum state has been taken in domain $\pi/2 < 0 < \pi$ to achieve real roots of K. The following expression includes the real constants α_1 and α_2. Since, the roots have been deduced for second quadrant the essential condition of the constant is $\alpha_2 > \alpha_1$.

$$(K-\alpha_1)(K-\alpha_2) = K^2 + (\alpha_2 - \alpha_1)K - \alpha_1\alpha_2 \tag{10}$$

Therefore, scattering rate equation (9) has been converted in the form of the factorials as follows with the assumption $\phi_{min} > \pi/2$. Hence, the first integral has been restricted to the limits from ϕ_{min} to π.

$$\frac{1}{\tau_i} = \gamma'\int_{\Phi_{min}}^{\pi}\int_0^{\infty}\delta\left((K-\alpha_2)(K-\alpha_1)\right)dK\,\sin\Phi\, d\Phi \tag{11}$$

Where, γ' is the constant prefactor which is given as

$$\gamma' = \frac{m^* e^2\omega p'}{2\pi\hbar^2}$$
$$p' = \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_s}\right)(N_0 + 1) \tag{12}$$

In above expressions, ε_∞ and ε_s are dynamic and static dielectric constants respectively, m* is the effective mass of GaN and e is the electron charge.

The scattering rate expression given in equation (11) provides the two solutions for $K=\alpha_1$ and $K\neq\alpha_1$ in the latter case no physical contribution occurs. But for $K=\alpha_1$, one observes significant contribution when solving the integral of equation (11) over phonon momentum K as the δ function reduces to zero. Thus, the simpler form of equation (11) under the condition $K=\alpha_1$ has been reduced to the following form. Hence, the determination of the scattering rate using equation (13) becomes refined for the better analysis of the electron transition in the superlattice structure as

$$\frac{1}{\tau_i} = \frac{\gamma'}{k_i}\left[\ln\left(k_i + \frac{\sqrt{k_i^2\hbar - 2m^*E}}{\hbar}\right) - \ln\left(\frac{\sqrt{2m^*E}}{\hbar}\right)\right] \tag{13}$$

The scattering rate has been observed from equation (9) to be a function of dielectric constant, which is having dependence on the wavelength, temperature and Aluminum mole fraction. The dielectric function dependent on mole fraction, wavelength and temperature is given by equation (14).

$$\varepsilon_r(E,x,T) - 1 = C(x,T) + \frac{A(x,T)}{E_g^{1.5}(x,T)} * \frac{2 - \sqrt{1+y} - \sqrt{1-y}}{y^2}$$
$$y = [E + i\Gamma(x,T)]/E_g(x,T) \tag{14}$$

$$C(x,T) = 2.49227*10^{-3}T - 1.80*10^{-6}T^2 - (0.74 + 4.61*10^{-3}T - 5.33*10^{-6}T^2)x$$

$$A(x,T) = [79.30 - 8.37*10^{-2}T + 6.73*10^{-5}T^2 + (18.99 + 0.13T - 1.76*10^{-4}T^2)x + 37.51x^2]eV^{1.5}$$

$$\Gamma(x,T) = [-8.69 + 4.13*10^{-2}T + (248.24 - 0.19T)x^2]*10^{-3}eV \tag{15}$$

In equation (14), E is the photon energy given by $(\hbar\omega)$ and equation (15) provides temperature dependence of dielectric function [16]. Thus, the scattering rate becomes dependent on wavelength and temperature.

3. Results and discussion

For the development of high-speed quantum well lasers, it is necessary to ensure both fast carrier transport to the wells and efficient capture into the quantum confined states. Carrier capture [6] into a quantum well is generally understood to proceed by inelastic polar optical phonon emission and carrier–carrier scattering. Quantum mechanical calculations predict resonances in the capture rate, which are dependent on the geometry and material composition of the well. Resonances are due to the capture of carriers in the continuum of unbound states that have high probability density in the well region. A superlattice structure provides the possibility of controlling the electronic and optical properties by varying the layer thickness and material compositions.

An increase in electron energy with the increase in barrier height and aluminum mole fraction has been attributed to the enhancement in electron confinement. The barrier height is greater than energy for confining the states in the well. Energy was found to increase in nonlinear manner with barrier height and the number of iterations needed to converge to higher value of energy is greater as shown in Fig. 1. To study the effect of material composition and layer thickness on the electron confinement, we have deduced the wave function intensity in 3-layer superlattice structure as shown in Fig. 2. The surface image of wave function intensities is obtained using MATLAB software as shown for three different values of energies in Fig. 2 (a). Brighter band at the center corresponds to peak intensity. Fig. 2 (b) shows waterfall images in which the wave function intensities are increasing and decreasing in nature due to the band alignment between well and barrier regions. The electrons are confined in well region because energy E remains less than the conduction band potential for different aluminum mole fraction 0.2%, 0.25% and 0.3%. The eigenenergy is found to be 0.206 5eV, 0.2520 eV, 0.2954 eV and barrier Height is calculated to be 0.3112 eV, 0.3956 eV, and 0.4827 eV respectively. The solution of Schrödinger equation consist of growing and decaying terms due to which wave function intensity increases in well region and decreases in barrier region. In three well superlattice structures, the wave function intensity is greater in central well for better confinement in the middle of structure than in other well regions. The motivaton behind introducing increasingly complicated structures is an attempt to tailor the electronic and optical properies of these materials for exploitation in devices. Here, we have studied the effect of eigen energy on the wave function intensity for the super lattice structure. The wave function intensity is maximum for the higher electron energy. The maximum intensity in the centre wells occurs due to the higher eigenenergy and barrier height.

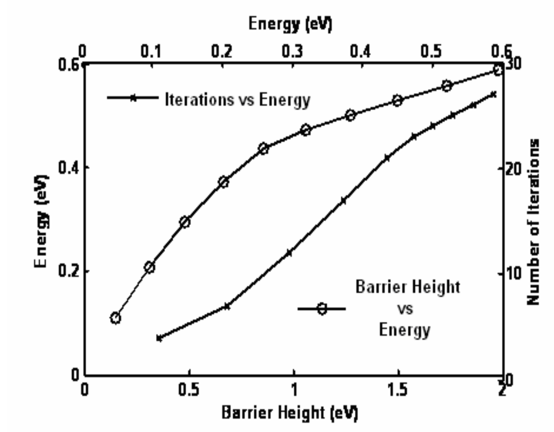

Fig. 1. Energy as function of barrier height and the iteration entail for the accuracy.

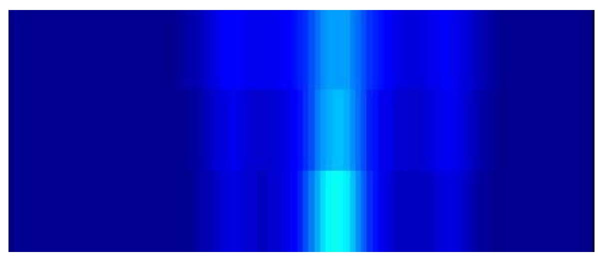

Fig. 2(a). Surface image of superlattice structure.

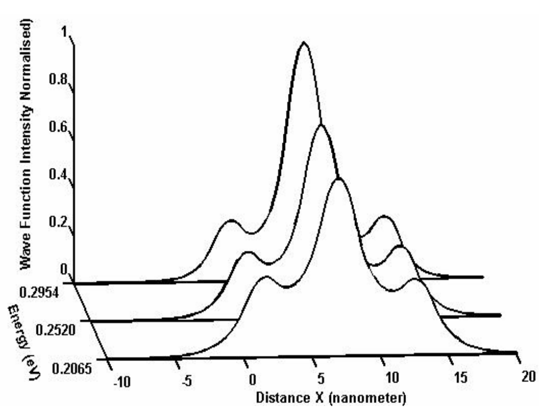

Fig. 2(b). The wave function intensity in 3-well superlattice structure.

Electron confinement is better in case of odd number of wells as revealed from the surface image of the wave function shown in Fig. 3 (a) and Fig. 3 (c) for the even and odd number of wells. The important observation made through Fig. 3 (a) is that in even number of quantum wells the two dominant bright bands appear for double quantum wells while, in Fig. 3 (c) only one strong band appears at the centre of superlattice structure. The significant analysis carried out through Fig. 3 (b) and Fig. 3 (d) shows that the device structure plays an important role in the electron confinement. In case of the even number of wells, the wave function intensity is greater when the number of the wells is less, while for the odd number of the wells the wave function intensity is observed to be higher for higher number of wells.

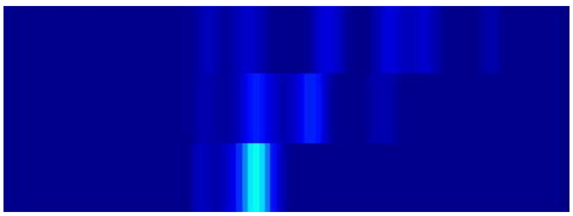

Fig. 3(a). Surface image for even number of wells in superlattice structure.

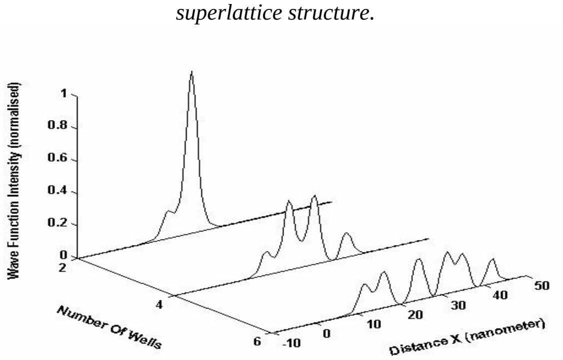

Fig. 3(b). Wave Function Intensity for even number of wells.

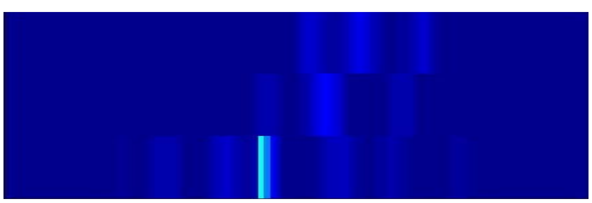

Fig. 3(c). Surface image for odd number of wells in superlattice structure.

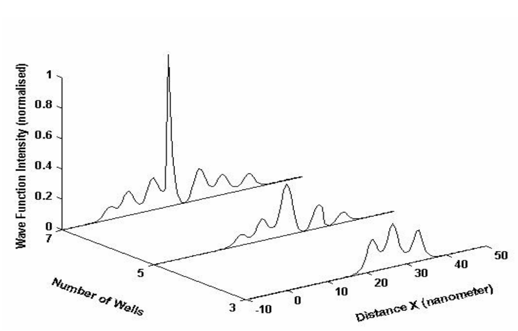

Fig. 3(d). Normalized wave function intensity for odd number of wells.

Fig. 4 shows the relationship between energy and transmission coefficient. The transmission coefficient becomes complex as energy increases. The wave function decays exponentially if E is less than V and transmission increases to unity in the barrier region. The electrons have a finite probability of passing through the barrier and appearing on the outside of the well, this phenomenon is known as quantum mechanical tunneling. One way of quantifying the proportion of electrons that tunnel through is in terms of transmission coefficient, which is define as the probability that any single electron impinging on a barrier structure will tunnel and contribute to the current flow through the barrier. Here, as shown in above result, it gives oscillatory feature. At the resonance energies, barrier structure appears transparent and has a maximum transmission coefficient. The wave functions of these states are localized between barriers and are often refers to as quasi-bound states. The analysis of electron tunneling is carried out through transmission coefficient, which affects to the electron hole recombination and the scattering rate, which is inversely proportional to the transmission coefficients.

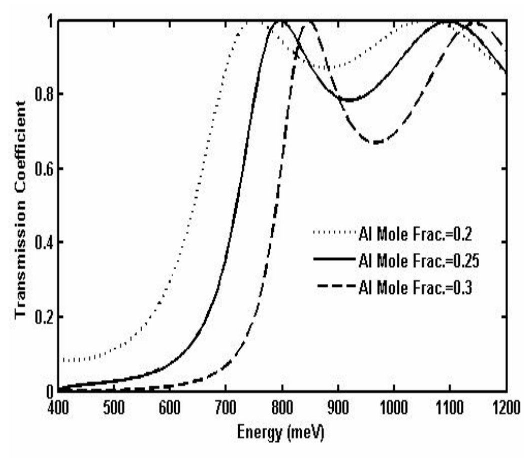

Fig. 4. Transmission coefficients as a function of energy.

The electron-phonon scattering is an important parameter and its analysis is very prolific for the optimization of electrical parameters. Electrical parameters such as barrier height and eigenenergy are very crucial for providing an efficient lasing action in a superlattice structure based laser diode. Fig. 5 shows the scattering rate as a function of wavelength and aluminum mole fraction. The increase in the wavelength results in increase of scattering rate. The increase in scattering rate is due to perturbation in the photon energy $(\hbar\omega)$, the photon energy decreases from 4.1421 eV to 3.1066 eV with increase in wavelength from 300 nanometer to 400 nanometer respectively. It is revealed that the scattering rate is more for the lower values of aluminum mole fraction, which is out come of smaller wave vector values in the well region.

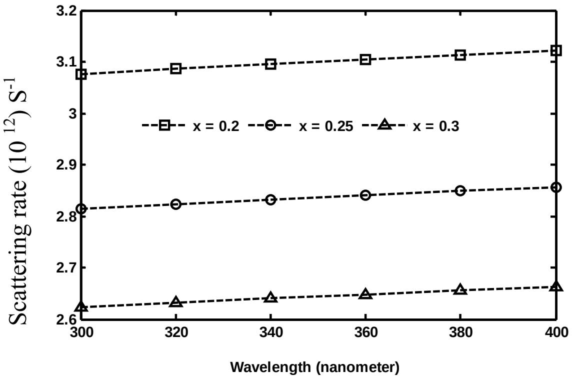

Fig. 5. Scattering rate dependence on wavelength.

The scattering rate deviation due to the variation in temperature and Aluminum mole fraction is observed from 2.4411×10^{12} to 3.6619×10^{12} per second as in Fig. 6. Both the parameters temperature and aluminum mole fraction are accountable for the perturbation in a barrier height of a superlattice. This perturbation in barrier height changes the energy state, which results in to a scattering of a carriers and phonon. Hence, the analysis of the scattering rate as a function of temperature and aluminum mole fraction has been carried out. The increase in temperature varies the energy state of conduction and valence band and significantly the temperature affects the Bose Einstein factor drastically. The Bose Einstein factor is phonon density, which increases with increase in temperature. The variations of electrical and optical parameters in a superlattice structure collectively increase the scattering rate.

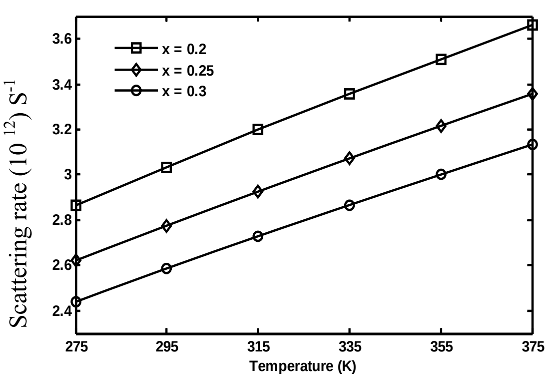

Fig. 6. Variation of optical phonon scattering rate with temperature.

The phonons, which usually dominate the scattering probability, in a polar semiconductor shift the electronic band states. The scattering due to longitudinal optical (LO) phonon significantly accountable for fastest carrier captures process in quantum structure based laser diode. The scattering occurs due to energy state perturbation; hence we had carried out analysis for the scattering rate for different eigenenergies. As shown in Fig. 7, the non linear dependence of scattering rate on eigenenergy has been observed. The increase in eigenenergy reduces the scattering rate, which is caused by increase in barrier height. The large barrier height opposes the tunneling of carriers, so the scattering rate decreases. The increase in carrier effective mass at the interface due to Eigen energy known as band – nonparabolicity significantly reduces the scattering rate in a superlattice structure.

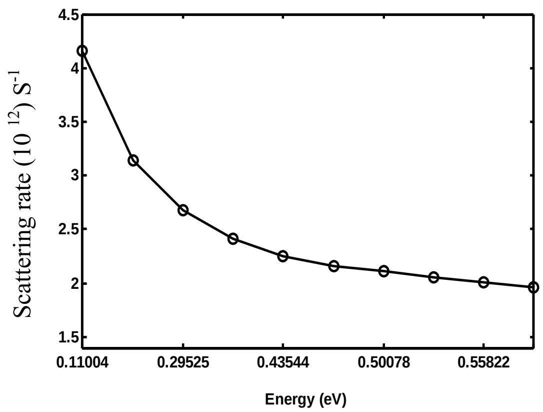

Fig. 7. Scattering rate dependence on Energy.

4. Conclusions

The fascinating behavior of interacting wave function intensity in case of superlattice structure has been studied for the electron transport and better electrical confinement. Dependence of scattering rate on material composition, temperature and wavelength has been investigated for the high speed GaN based laser. Since barrier thickness is very less in case of superlattice, carrier tunneling alters the transport properties and leads to minibands formation. Therefore, the transmission coefficient has been estimated for the different values of energy and material composition. The peak transmission coefficient for the lower mole fraction (0.2) is obtained for the lower value (750 meV) of eigenenergy when the barrier height is kept constant. The brighter spots in surface image of wave function clearly depict better confinement in the innermost well of superlattice structure. The scattering rate decreases with the increase in Aluminum mole fraction and increases linearly with the increase in temperature considerably. The effect of wavelength on scattering rate is found to be very minimal. It is observed from the results that the scattering rate increases linearly with the increase in wavelength due to the increase in eigenenergy and static dielectric constant. Our analysis explores optimization of physical parameters of GaN superlattice structure to provide useful physical insight for the development of high-speed lasers.

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