Chapter 2

Electronic Band Structure of Quantum Cascade Laser

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Additional information is available at the end of the chapter

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Abstract

Multiple quantum well structure is the subject of theoretical and experimental research over the last two decades due to the possibility of making novel electronic and optoelectronic devices. The phenomenon of resonant tunneling makes it a prime candidate for all tunneling-based quantum devices with one-dimensional confinement. THz laser design using multilayered low-dimensional semiconductor structure is one such example, where miniband formation and its energy difference with lowest quantum state play crucial factor in governing device performance. Quantum cascade laser (QCL) is one of such candidate, which speaks in favor of research using multiple-quantum-well (MQW) structure. In the proposed chapter, transmission coefficient of multiple quantum-well structure is numerically computed using propagation matrix technique, and its density of states is calculated in the presence and absence of electric field applied along the direction of quantum confinement. Absorption coefficient is also calculated for its possible application as optical emitter/detector. Based on the electronic and photonic properties investigated, electronic band structure of the quantum cascade laser (formed using the MQW structure) is computed. Formation of miniband is tailored with variation of external bias is shown.

Keywords: multiple quantum well, electronic band structure, quantum cascade laser, miniband, band nonparabolicity, electric field

1. Introduction

Research in the area of nanostructures, more precisely on optoelectronic and photonic devices, has progressed in the last few years as novel and unique properties are emerged, which may substantially be able to solve the complex existing problems in the domain of communication and information processing [1–3]. Owing to the synchronized development in material science and nano-fabrication technique [4, 5], in-depth investigations in both experimental and theoretical ways on semiconductor nanostructures lead to the possible realization of novel electronic [6, 7] and photonic [8, 9] devices. Quantization of energy states in low-dimensional semiconductors along different directions leads to the formation of quantum well, wire or dot, which are characteristically different from their bulk counterparts. It would be very difficult today to imagine solid state physics without semiconductor heterostructures, more precisely double heterostructures. The genesis of semiconductor electronics is from the feasibility of conductivity tuning by external impurities by means of doping. This feature along with the concept of non-equilibrium carrier injection helps to breed the semiconductor industry. Heterostructures provide the potential means for solving the far more general problem of controlling fundamental parameters in semiconductor crystals and devices, such as the width of the bandgap, the effective masses and mobilities of charge carriers, the refractive index and the electron energy spectrum. These structures can be used as infrared detectors [10, 11], which has immense applications in medical [12], defense [13] and communication [14] fields. Characteristics of these IR devices may be studied from absorption coefficient profile, and thus its accurate determination becomes very important from device design point of view.

To understand the electronic and optical properties of the nanostructures, computation of their eigenstates is very essential along with density of states profile [15]. Among the quantum structures, quantum well is extensively researched in the last decade because of computational advantages [16–18] and also eases of fabrication [19]. Multiple quantum well structures are subject to theoretical and experimental research in last two decades because of the resonant tunneling phenomenon [20], and novel photonic devices are already designed as transmitter [21] and receiver [22] applicable in nanoelectronic domain. By virtue of quantum engineering, electronic energy states are tuned by suitable application of external excitation in this complex multilayered structure as per the requirement by tailoring the electronic and optoelectronic properties of quantum heterostructures. One such example is the THz laser design with low-dimensional semiconductor structures [23] with multiple layers, where miniband formation and its energy difference with lowest quantum energy state (lowermost energy band) play crucial factor in governing the device performance [21] as optical transmitter. This is one typical semiconductor laser with room temperature operation at IR range, with good peak output power and CW mode of operation [24]. Operation of this unipolar device is based on quantum tunneling and intraband transitions, and formation of miniband critically depends on layer dimensions, their compositions and periodicity [25]. The layer thickness is essentially responsible for determining the wavelength of emitted radiation, as compared to the other semiconductor-based lasers where bandgap of the material determines the wavelength. Thus, accurate determination of electronic band structure of quantum cascade laser (QCL) is very important for theoretical researchers from the point of view of optoelectronic application.

2. Literature review

Semiconductors form the basis for the most modern information processing devices. Electronic devices, such as diodes, bipolar junction transistors and field effect transistors, drive modern electronic technology. Optoelectronic devices, such as laser diodes, modulators and detectors, drive the optical networks. In addition to devices, semiconductor structures have provided the stages for exploring questions of fundamental physics. Quantum Hall effect and other phenomena associated with many-body effects and low dimensions have been studied in semiconductor structures.

Theoretical and experimental researches are so far carried out on the abrupt semiconductor heterostructure composition, precisely the combination of GaAs and AlGaAs. The popularity of this material system is due to the fact of near-perfect match between the GaAs and AlAs binary components. Interestingly, bandgap of GaAs is not suitable for the application of IR detectors, optical transmitter design at infrared region, long-wavelength optical sources and signal processing devices. Several moderate and narrow gap materials are already emerged out for signal processing applications and also for sensing elements in electrical circuits. To name a few, InSb, InAs and GaSb are the materials on which researchers are conceded, and these are categorized as emerging narrow gap materials. Their acceptance of making quantum devices is primarily due to the higher mobilities, bandgaps correspond to the infrared region of electromagnetic spectrum, saturation drift velocities and very low effective mass. Combination of these properties provides higher quantum confinement energies. Higher eigenenergies lead to the possibility of exhibiting mesoscopic property, that is, Aharonov-Bohm effect and Coulomb Blockade effects at higher temperatures.

One of the most interesting research areas in the low-dimensional semiconductor heterostructure is to study novel electronic and photonic properties, which already initiate some technological revolutions [26]. Quantum well, wire and dot are the examples of nanostructure, where quantized dimension has the order of de-Broglie wavelength. Quantum well is the most popular one, can be coupled with external world by means of resonant tunneling. This phenomenon leads the various researches in the last two decade for low-bias applications. Freire [27] calculated multiple-quantum-well (MQW) laser parameters for a dispersion supported transmission system. At very high transmission speed (20 Gbit/s), optical system is simulated for laser parameters using multiple-quantum-well (MQW) system. For strained layer MQW laser, simulation parameters are precisely estimated through signal intensity modulation (IM) response model in order to obtain response curve for communication application. Recently, Taghavi [28] showed that transistor performance can be improved if isolated well is replaced multiple well system. Significant enhancement in device performances is anticipated when the MQW structure is properly designed. Stöhr et al. [29] experimentally characterized electro-optical modulators and switches based on MQW-structure. It can also be used for making quantum cascade laser (QCL) [30], resonant tunneling diode (RTD) [31], resonant tunneling transistor (RTT) [32], quantum well infrared photodetectors (QWIP) [33], etc., which have greater efficiency compared to their bulk counterparts. QCLs are preferred for broadband tuning, RTD and RTT for digital circuits and negative resistance devices. QWIP is used for night vision and medical diagnostics.

Transmission coefficient needs to be computed for analysis of quantum well structures, and also for studying tunneling probability by various numerical approaches like variational method [34], Airy's function approach [35, 36], finite element method [37], transfer matrix technique (TMT) [7, 38–40] and weighted potential method [41]. A comparative analysis among these methods reveals the fact that TMT is one of the best effective procedures. For multibarrier structure analysis at biasing condition, a theoretical estimation about transmission coefficient [17, 38, 42–45] gives corresponding estimation of eigenstates. Significant theoretical contributions on quantum well multilayered heterostructures deal with resonant tunneling mechanism, which is obtained based on accurate solution of the Schrodinger equation subject to the application of uniform magnetic field or constant electric field applied along the perpendicular direction of confinement or along the direction of confinement. Adopting transfer matrix technique, the transmittivity of the multilayered structure is calculated with incident electron energy in the presence or absence external field. Simulated results show good agreement with other existing model, and also with bound-state energies. Based on these calculations, a new class of resonant tunneling superlattice devices has been designed.

Miller [46] investigated the effect of band nonparabolicity on eigenenergies using Kane's two-band model, later considered as a function of material parameters by Hiroshima [47]. Nonparabolicity is accounted for calculation of transmission coefficient by Palomino-Ovando [48]. He used transfer matrix technique (TMT) with nonparabolic dispersion relations for conduction band electrons, which is incorporated in the modified Schrödinger equation; and 2 × 2 matrices are generated. This method is implemented to the study of quasi-periodic semiconductor heterostructures maintaining Fibonacci series property. Miniband formation is observed and amplitudes of resonant tunneling peaks are measured. Results are compared with that obtained for parabolic case to justify the importance of nonparabolic deviations in $Al_xGa_{1-x}As/GaAs$ superlattices.

Multiple quantum well structure is a low-dimensional semiconductor nanostructure which is coupled through the external world by means of resonant tunneling; and based on this physical insight, several novel electronic [31, 32] and photonic [30–33] devices are fabricated which is far superior to their bulk counterparts. The analysis of resonant tunneling diodes was carried out with submicron-sized mesa structures along with contacts at both the terminals in order to measure the current-voltage characteristics in the bistable regime at room temperature. Investigation reveals the noise-triggered firing of spike-like signals from the RTD's biased dynamically, and they act as universal logic gates with reconfigurable property for mini voltage changes ranging from a few mV at the input coordinates. It has also been shown that the RTD junction can be easily integrated to arrays of multiple inputs and has thus the potential to mimic neurons in nanoelectronic circuits.

RTD is already used with slot antenna. With an offset-fed slot antenna, the device is placed at a specified distance w.r.t. slot center, and used in oscillator with considerable output power (100–200 μW) at frequencies of 430–460 GHz. If the distance from the slot center is kept 45 μm for 100 μm long antenna, then 200 μW output power can be obtained (which was the maximum power) at 443 GHz for a single RTD device with a peak current density of 18 mA/μm^2. This opened the door of possible application of quantum well–based devices for communication application at both transmitting and receiving ends. Simultaneous optimization of antenna length and position of quantum device enhances the output performance. Based on this novel investigation and superior performance, a large-format (640 × 512) voltage-tunable quantum-well (QW) infrared photodetector focal plane array (FPA) is designed for both the mid- and long-wavelength infrared (MWIR and LWIR) bands for the sole purpose of imaging applications. Using MBE technique, 8 well MWIR stack with AlGaAs-InGaAs composition and 16 well LWIR stack with AlGaAs-GaAs system are developed and series connection is made between them which provided excellent voltage-tunable spectral response property. Results show a very well redshift of peak responsivity (4.8–8.4 μm, within IR range) with increase of bias within the applicable limit as determined by commercial IC's.

Biasing effect on the lowest three eigenstate of four-barrier three-well MQW structure assuming realistic band structure has been studied by accounting conduction band nonparabolicity. Only first-order nonparabolic effect is considered, and transfer matrix technique is used to solve the problem. $GaN/Al_xGa_{1-x}N$ material composition is assumed for simulation purpose, as the device is aimed to design optical transmitter. The method is well established [38, 39], and results obtained by using TMT are quite accurate when compared with the results obtained using other methods.

Semiconductor nanostructure is the topic of research in the last decade due to its possible novel applications in the field of electronics [9] and photonics [49]. It has been studied that the photonic crystals composed of at least two different semiconductor heterostructures exhibit resonant photonic states, and the composition may be termed photonic double quantum well (PDQW). The heterostructure is schematically denoted as ....Q/P/Q/P/Q...., where P and Q act as photonic wells and barriers depending on their refractive indices, and thus bandgaps, respectively. The resulting band structure exhibits photonic bandgap, similar to the electronic bandgap in semiconductor and dielectric, and photons having energy within that electromagnetic forbidden region could not propagate. This leads to the discrete quantized states. Mathematical modeling has already been carried out for the transmission coefficient of the PDQW heterostructure using both transfer matrix method and plane wave propagation method, and it has been found that within the photonic wells, resonant states exist in split pair mode. This is due to the fact that coupling between degenerate states due to the propagation of forward and backward waves inside this electromagnetic structure, resonant states originate, and it is shared by the both layers of the unit block. Simulation study reveals that resonant states appear as single peak in the transmission spectrum when the energy is within the range of bound photonic state, and then separation distance between the adjacent photonic quantum wells is very large. However, with reduction of the thickness of the sandwiched barrier layer, energy-splitting effect is observed, which is represented by two adjacent resonant peaks in the transmission profile. This realization makes the possible operation of the device as switch single and double transparent states. Similar to the electronic MQW system, in the photonic structure also, number of resonant states can be tailored by varying the dimension of the photonic wells and barriers. Also by increasing the contact barrier widths, quality factor of transmitted peaks can be significantly improved. Researchers are already performed to utilize this property in developing optical filter, transmitter, switch, quantum information processing, receiver and devices, which are suitable in all-optical integrated circuits. The major unique feature if these devices are they are pure photonic devices compared with the existing optoelectronic devices. Quantum confinement is made by reducing the device dimensions of the order of electron wavelength along one, two or three dimensions; results in quantum well, wire or dot, respectively. These quantum systems are usually coupled with the external world through tunneling barriers, which vividly reflect the dominance of the quantum effects to understand the physical properties of heterostructure devices; and the discrete electronic states become resonant one.

Calculation of these eigenstates thus becomes very essential to study the electronic and opto-electronic behavior of the nanodevices [50, 51]. For determining eigenstates, BenDaniel-Duke boundary condition is incorporated in order to consider the effect of effective mass mismatch at different hetero-interfaces, as well as to consider the conduction band discontinuity, which leads to the quantum well potential height. Difference of bandgap gives the second consideration, whereas numerical calculation reveals that results are erroneous when constant effective mass is considered. This signifies the effect of boundary condition at numerical estimation. Structural parameters (in terms of thicknesses of the layers and number of layers) are important players in tuning the energy values. Simulations are also performed in the presence and absence of electric field. In most of the literatures, $GaAs/Al_xGa_{1-x}As$ material composition is considered to understand tunneling probability.

Material compositions of the heterostructures also have a profound effect on the transmission characteristics under resonance condition. Among the quantum structures, quantum well is already studied a lot [16–52] because of computational advantages for analysis and also eases of fabrication [17, 53]. Density of states is one of the very important parameter of nanostructure as it provides the eigenstates from lowermost value [54]. Its profile is changed by application of external field; thus a comparative study my reveal the possibility of low-bias applications through resonant tunneling. Work on density of states of quantum well is carried out by researchers in presence of inelastic scattering [55] along with computation of transmission probabilities. It has been shown that shot noise in a resonant tunneling diode biased in the negative differential resistance regions of the I–V characteristic is enhanced with respect to 'full' shot noise. Experimental results suggests that profile of density of states function for particular type of quantum well system is the governing cause of the so-called noise effect, physically controlled by electron-electron interaction through Coulomb force. Numerical results are also presented from the above-mentioned theory, which are in close proximity with the experiment. This ensures that the model presented is accountable for the relevant physics involved in the phenomenon.

Step-like shape of the density of state (DOS) profile is used to study the characteristics of heterostructure well laser [56]. For finite-barrier quantum well, it differs from what obtained for infinite well problem [57]. The results presented in this chapter, obtained by applying the correspondence with the bulk density of states (DOS), indicate that the DOS in finite-barrier quantum wells differs substantially from the conventional 2D DOS calculated for infinite-barrier quantum wells.

Peak of the DOS is analytically related with the occurrence of resonance [58] along with transmission and reflection phase times. Existence of quasi-bound states is observed from DOS plot [59] for specially designed rectangular well structures. Numerical calculations have been presented, which substantially prove that electron states are present in the continuous part of the spectrum for different quantum well devices irrespective of well geometry. Initial works are carried out on rectangular potential profiles. Necessary boundary conditions for creation of these quasi-states are theoretically investigated. At very high energies in conduction band, existence of these quasi-bound states with spatial localization is determined. The results can be very useful in design of semiconductor optoelectronic devices whose working principle will be based on continuum bound states.

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With the emergence of nanoelectronic devices as the possible replacement of existing VLSI technology, the need of resonant tunneling device in sub-micron domain becomes very important for low bias application point of view, and theoretical research for accurate design of these structures leads to the invention of novel electronic and optoelectronic properties. Ultrathin semiconductor quantum devices are now the interests of research where quantum well, wire and dot have already realizable because of the advancement of microelectronics technology. For accurate estimation of resonant tunneling, displacement of energy levels from the band-edge should be considered; hence, realistic band structure plays a very important role for different material parameters. This leads to the better computation of intersubband transition energy for optical emitter/detector design [50, 60]. Intersubband transition energy is computed for core-shell (normal and inverted) quantum dots (CSQD) of cubic and spherical geometries by solving time-independent Schrödinger equation using finite-difference technique. Sparse, structured Hamiltonian matrices of order $N^3 \times N^3$ for cubic and $N \times N$ for spherical dots are produced considering N discrete points in spatial direction. The matrices are diagonalized to obtain eigenstates for electrons. Computed results for the lowest three eigenstates and intersubband transitions are shown for different structural parameters taking GaAs/$Al_xGa_{1-x}As$-based CSQD as an example. Reduction of subband transition energy is observed with increase in core thickness. A comparative study reveals that spherical CSQD exhibits higher transition energy between any two subbands than that is demonstrated by cubic CSQD of similar dimension and equal material composition. More interesting phenomenon is observed for inverted core-shell structure. In this case, transition energy monotonically decreases for cubic dot, while it is increased for spherical dot with enhancement in core size. These devices are utilized as optical emitter/detector due to the wider range of tuning in intersubband transition through tailoring dot dimensions.

Miller investigated the effect of conduction band nonparabolicity on eigenstates using Kane's two band model. Hiroshima showed the importance of material parameters to evaluate the same. Nelson introduced the energy-dependent effective mass theory [61] following Ben-Daniel Duke boundary condition for precise estimation of carrier energies. Palomino-Ovando extended the analysis for superlattice structure [62] where energy was calculated form transmission coefficient peaks. The work of Li in determining the electron states in multilayer semiconductor quantum devices plays a significant role. He showed that finite element method can effectively be used for near accurate determination of these electron states. Moreover, he emphasized on the importance of band structure consideration and showed the effect of Kane type conduction band nonparabolicity over the carrier states. For two different material compositions, the result is presented in tabular form.

This work is incorporated in modulator design [63]. Using multiple quantum well structures, authors show that spatial light modulators can be designed. Reflectance levels are calculated for 128 × 128 pixels ternary spatial light modulators with 10 KHz operating frequency. It is shown that single reflectance level can be duo with just a 180° phase difference. Structural design parameters of the modulator will play important role in determining the performance of the device.

Due to the rapid advancement in microelectronics technology [64, 65] in the last decade, research in the domain of semiconductor nanostructure has been carried out to a great extent by both theoretical [4, 66] and experimental workers [5, 6]. Quantum well waveguide is fabricated by ion implantation technique using InGaAsP/InP material composition. Multilayer structure is developed for waveguide gratings precisely for the application at CWDM wavelengths. Reactive ion etching technique is utilized to reduce the roughness below 5 nm (experimental results show surface roughness is approximately 2–3 nm). Significant findings emphasize the importance of this quantum device as cross talk between adjacent channels goes below −10 dB level in the transmission spectra of the waveguide. Moreover, insertion loss of the grating becomes less than 5 dB, which is another major advantage for communication application.

Heterostructure light emitting diode is made by InGaN/GaN composition using MOCVD technology. Strucutre is developed over $LiAlO_2$ (100) substrates consisting of multiple quantum well with five wells along with GaN p-n junction. Colors of the output emission (generally blue or green) depend on the indium composition of InGaN layer of the MQW structure. Proof of quantum well interface is experimentally obtained by third-order satellite peaks. These are measured by high resolution x-ray diffraction set-up. Good performances are reported in various literatures; for example, 3 mW output power is achieved for 800 × 800 μm^2 blue LED device with 200 mA input current. It is also experimentally observed that for green and blue LED's with InGaN/GaN composition, electroluminescence (EL) spectra suggest that peak wavelength almost saturates at some precise positions of the spectrum with enhancement of injection current. Henceforth, it may very easily be concluded that polarization fields are totally absent in the active region of the structure.

Spin-photonic semiconductor devices are the another novel class of quantum well based devices, which are researched in recent days due to the ability of controlling electronic and optoelectronic properties using the spin of conduction electrons. The two most promising examples of these devices are spin-switches and spin-vertical-cavity surface-emitting lasers (spin-VCSELs). Experimental investigation showed that circularly polarized laser with very high degree of circular polarization (0.96) at room temperature is obtained using GaAs/AlGaAs multiple quantum well vertical cavity surface emitting laser structure where spin relaxation time is very high (0.7 ns). Furhter works with the same structure also showed that carrier lifetime and electron spin relaxation time can be tuned by design parameters. This also modifies the lasing characteristic. Orientation of the wafer plane plays a very crucial role in this regard. All the experimental results are obtained for <110> wafer. Investigation is also conducted on p-i-n structure with similar material composition. Result showed that remarkable reduction of spin relaxation time can be obtained (4–0.3 ns) when the quantum well structure is subjected under external electric field applied along the direction of well width at room temperature. To understand the electronic and optical properties of the nanostructures, computation of their eigenstates is very essential along with density of states profile [16]. Among the quantum structures, quantum well is extensively researched in the last decade because of computational advantages [7, 8, 67] and also eases of fabrication [9].

Transfer matrix technique (TMT) and propagation matrix method (PMM) are the two most suitable cost-effective methodologies for the analysis of wave function profile, confined energy states and transmission coefficients in superlattice nanostructures. There are other numerical

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methods like finite element method (FEM), finite difference method (FDM) but the complexity of the programming makes the computational time larger. However, these later methods are very accurate regarding the precision of the obtained results. Material composition for the ternary or quaternary heterostructures plays the bigger role along with Ben-Daniel Duke boundary conditions for determining the basic electrical properties of multilayered structures. Structural parameters within fabrication limit showed the variation of electronic (eigenenrgy, density of states, for example) and optoelectronic (absorption coefficient, oscillator strength, for example) properties of this superlattice structure which are pivotal in analysis of further complex structures. Otherwise multiple quantum well structures become a superlattice structure when width of the barrier layer between adjacent quantum wells is reduced to very small dimension, and this ensures the beginning of resonant tunneling through intermixing of the wavefunctions between the quantum wells. This provides a new insight in the nature of interacting wave functions for thin barriers. Number of wells in this computation becomes also important along with the structural parameters and material compositions. Different iterative methods are implemented for complex geometrical structures. Doping of the wells is taken into account through self-consistent solution of Schrödinger and Poisson's equations.

Thus, a comprehensive analysis of electronic and optical properties of MQW structures will make the foundation for understanding the quantum cascade laser. Its principle of operation is essentially dependent on the band structure, layer thickness is primarily responsible for determining the wavelength of emitted radiation, as compared to the other semiconductor based lasers where bandgap of the material determines the wavelength. Thus accurate determination of electronic band structure of quantum cascade laser is very important for theoretical researchers from the point of view of optoelectronic application.

3. Transmission coefficient of multiple quantum well structure

For analyzing electrical property of MQW structure, first transmission coefficient is calculated by considering a three-well four-barrier structure with rectangular potential profile configuration having GaN as well layer and $Al_xGa_{1-x}N$ as barrier layer. It is observed that by increasing well width, transmission probability increases. This is due to the fact that by increasing tunneling dimension of the well, quantum confinement decreases, so transmission can be achieved at lower energy values. By changing the material composition of barrier material, it is observed that transmission coefficient decreases with increase of Al mole fraction. It is plotted in **Figure 1**. This is due to the fact that by increasing Al percentage, potential height increases and effective mass mismatch at the junction also increases. This increases quantum confinement, which increases the eigenenergy. By increasing the thickness of the contact barrier, transmission probability reduces, whereas it increases if contact barrier thickness is reduced compared to that of the internal barriers. This is shown in **Figure 2** for both parabolic and nonparabolic band structures. By increasing number of wells, it is observed the eigenvalue reduces, and ultimately becomes constant for higher numbers, as evident from **Figure 3**. Eigenvalue increases with increase of material composition, as suggested from previous results, plotted in **Figure 4**. Obviously, for nonparabolic band structure, eigenenergy is less compared to the ideal parabolic concept. The variation is almost linear, and the gap reduces with increase of al mole fraction.

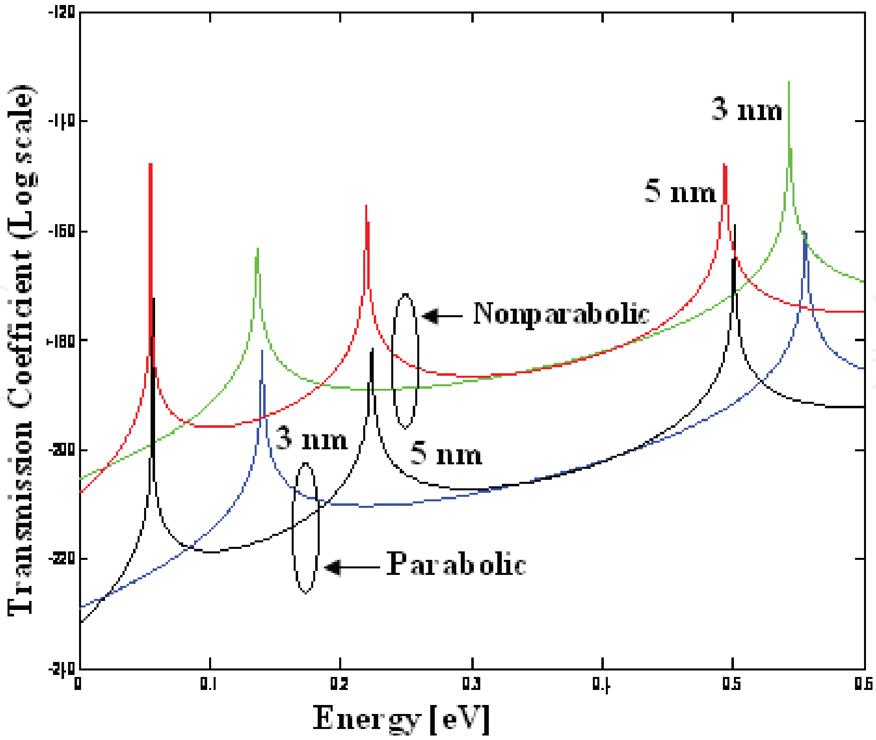

Figure 1. Transmission coefficient with energy for different barrier material composition for both parabolic and nonparabolic structure.

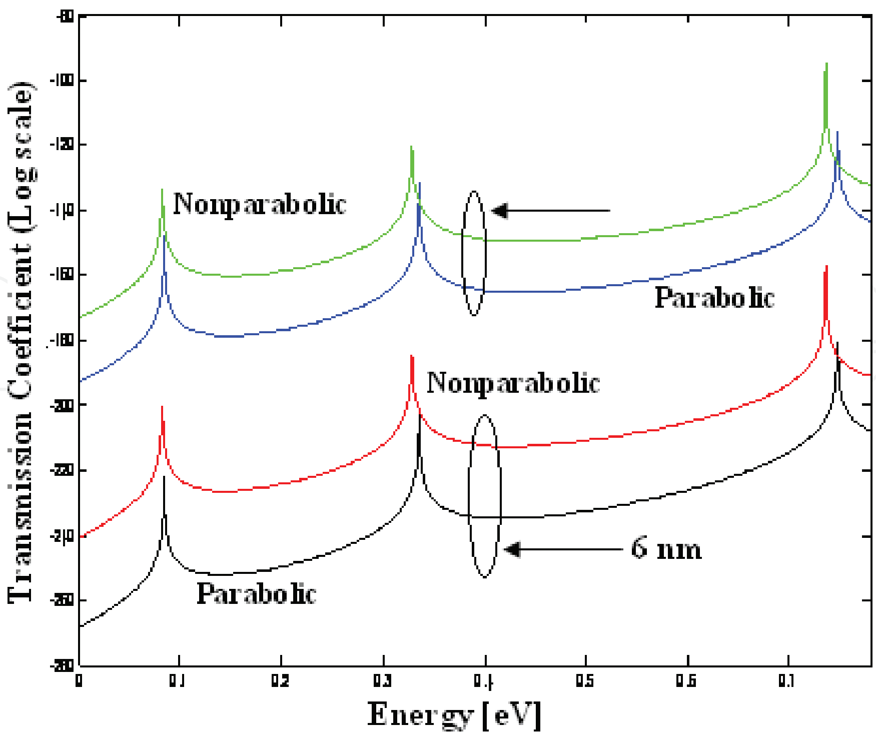

Figure 2. Transmission coefficient with energy for asymmetric barrier width for both parabolic and nonparabolic structure.

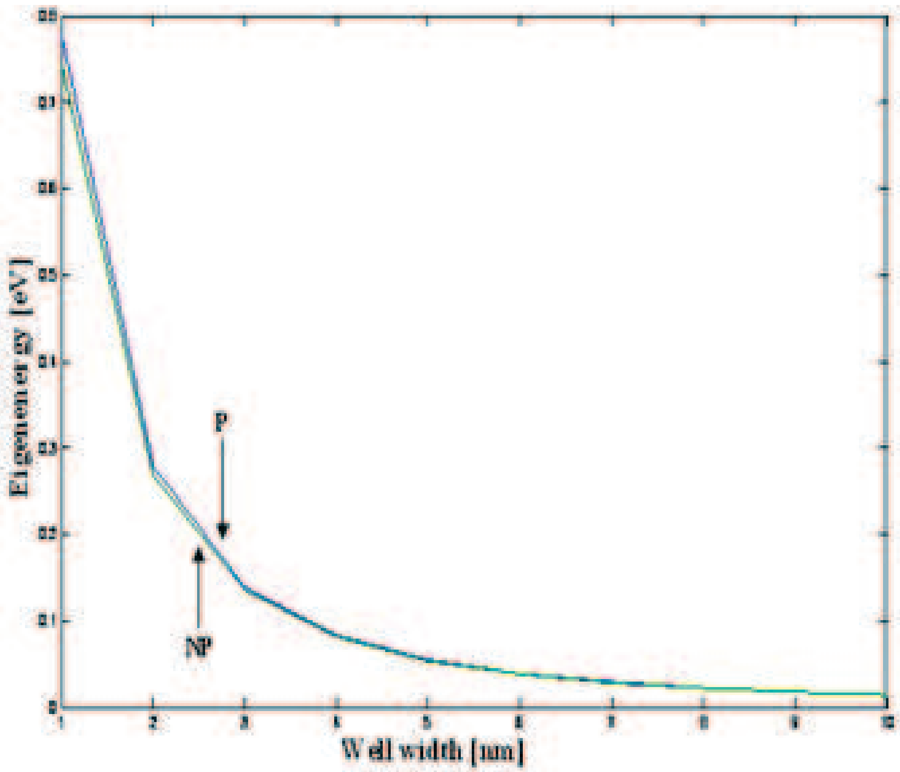

Figure 3. Eigen energy with dimension of well for both parabolic and nonparabolic structure.

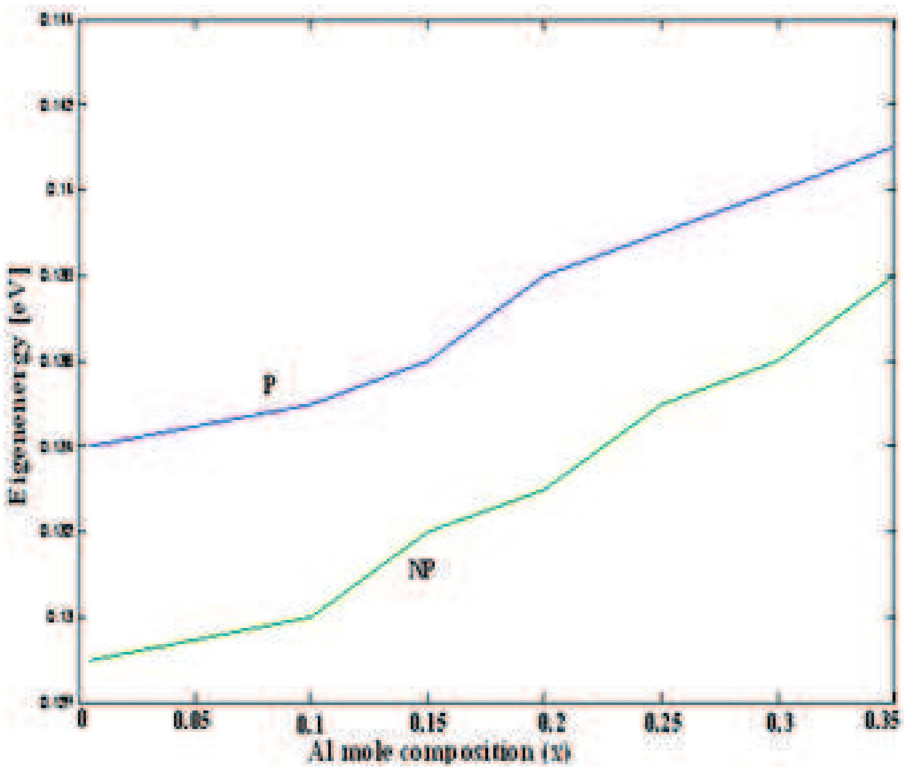

Figure 4. Eigen energy with barrier material composition for both parabolic and nonparabolic structure.

4. Density of states of MQW structure

In **Figure 5**, density of states (DOS) is plotted for lowest two eigenstates with different well widths. It is observed from the plot that by increasing the well width, eigenenergy appears at lower energy values due to the reduction of quantum confinement. It may also be seen that higher bandgap system provides eigenstate at lower energy range. Hence, optical device based on GaN/AlGaN system can be tuned at lower bias. Also due to closeness of first two energy levels in this composition, intersubband transition energy is higher for InAs/GaInAs system, which makes it efficient candidate for high frequency laser.

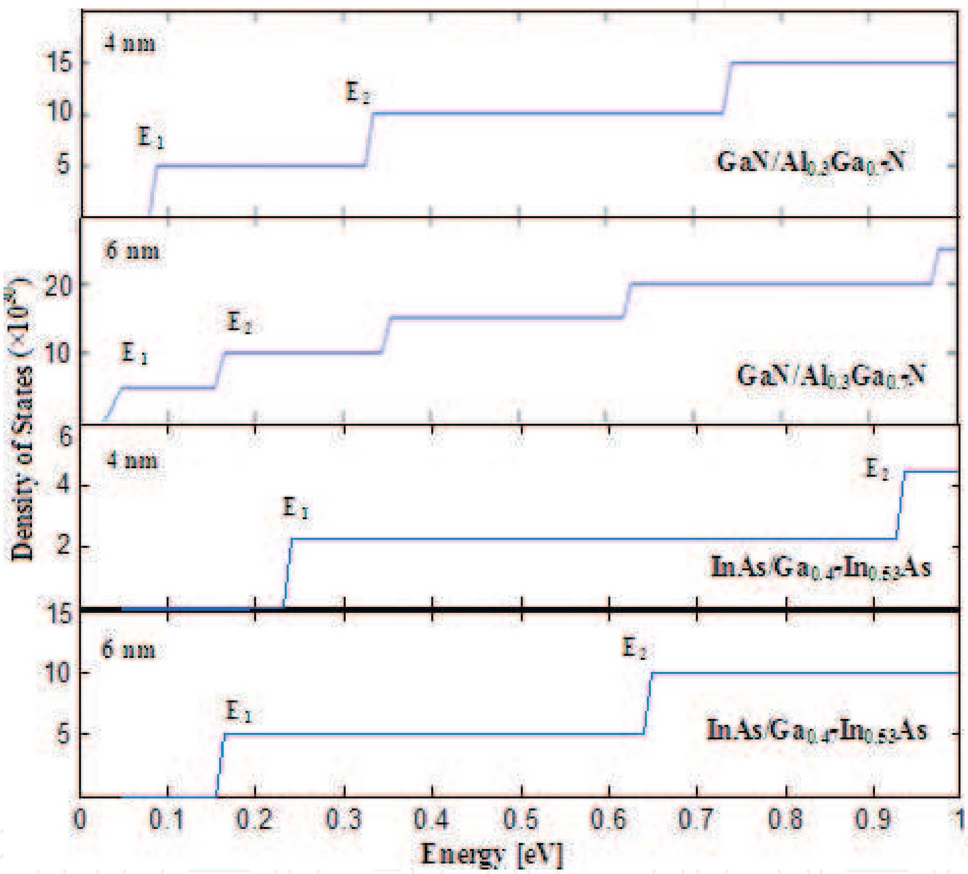

Figure 5. Density of states for the lowest two eigenstates for different well widths and different material compositions with nonparabolic dispersion relation.

Figure 6 shows the comparative study of DOS in presence and absence of electric field for InAs/GaInAs material composition. From the graph, it may be noted that application of transverse field lowers the magnitude of eigenstates irrespective of dispersion relation considered for simulation. Results are also compared with overestimated parabolic assumption. It may be observed from the comparison that incorporation of band nonparabolicity reduces the eigenvalue. Hence, for fine wavelength tuning purpose to design photonic transmitter/detector, realistic band structure consideration plays a vital role.

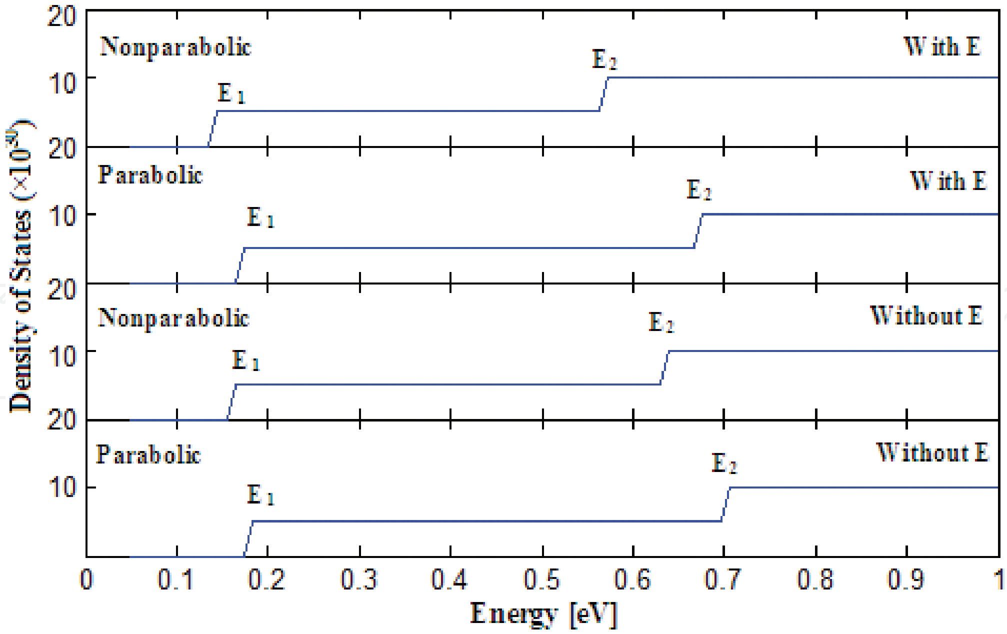

Figure 6. Density of States for the lowest two eigenstates in presence of absence of electric field for nonparabolic and parabolic structures.

By varying the material composition of barrier layers, it is observed that quantum states appear in higher energy values with increase of GaN mole fraction. The result is shown in **Figure 7**. This is because with increase of x, mismatch of effective mass increases as well as the conduction band discontinuity. This enhances the quantum confinement. Hence, eigenenergy increases. This is reflected via density of states plot.

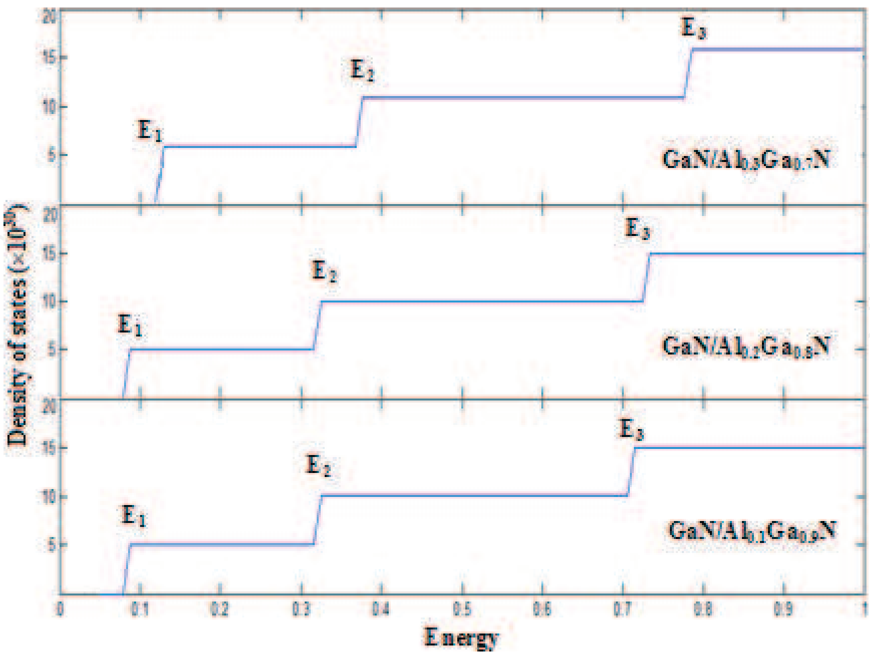

Figure 7. DOS of superlattice with different material compositions in absence of field considering band nonparabolicity.

5. Absorption coefficient of MQW structure

Absorption coefficient is calculated as a function of operating wavelength for different well width, as shown in **Figure 8**. For lower well dimension, it is found that the absorption coefficient value is less compared to the higher well dimension. Again, when the energy difference between the bands increases, interband transition energy increases. This reduces the peak of absorbance amplitude, provided half-width at half-maximum is kept constant throughout the simulation.

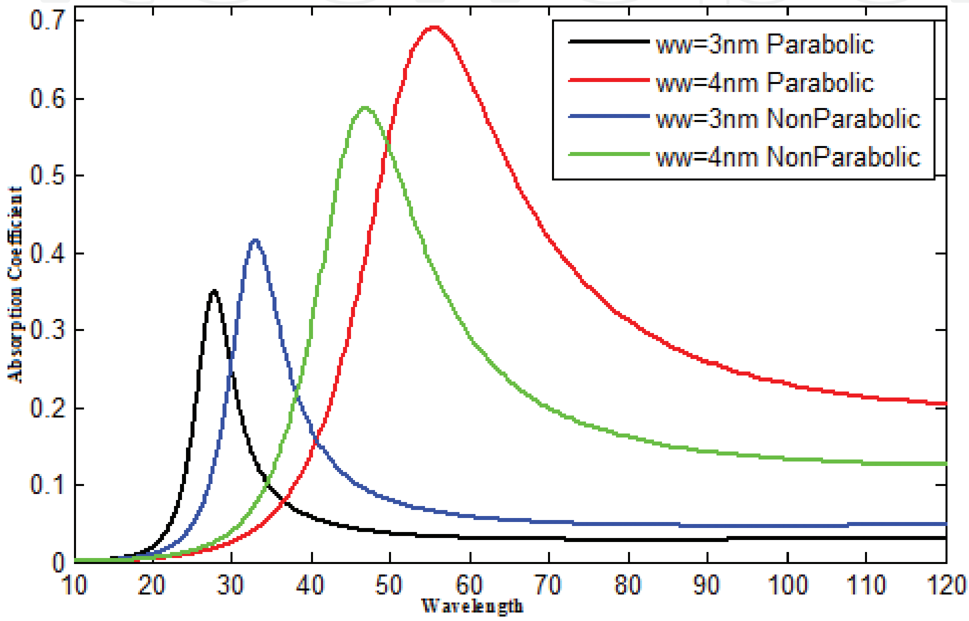

Figure 8. Absorption coefficient for different well dimension with wavelength variation for parabolic, nonparabolic dispersion.

With increase of well dimension, redshift is observed for all the profiles corresponding to the transition energies; also peak value is shifted rightwards and the wavelength value increases. When the parabolic and nonparabolic dispersion relation is considered for same well dimension the peak value is greater for lower well dimension nonparabolic case. But with change in eigenenergy, for higher well dimension the parabolic relation gives a higher absorption peak value. Thus the nonparabolic dispersion relation takes the priority for simulation.

With parabolic and nonparabolic relations into consideration the material composition is varied in accordance with the wavelength. The absorption coefficient profiles are depicted in **Figure 9**. For parabolic dispersion, the transition energies are low, so the absorption peak values are less compared to that of nonparabolic case. Also for higher material composition the shift in absorption value is considerable. The peak absorption values are greater for higher material composition and also for nonparabolic dispersion.

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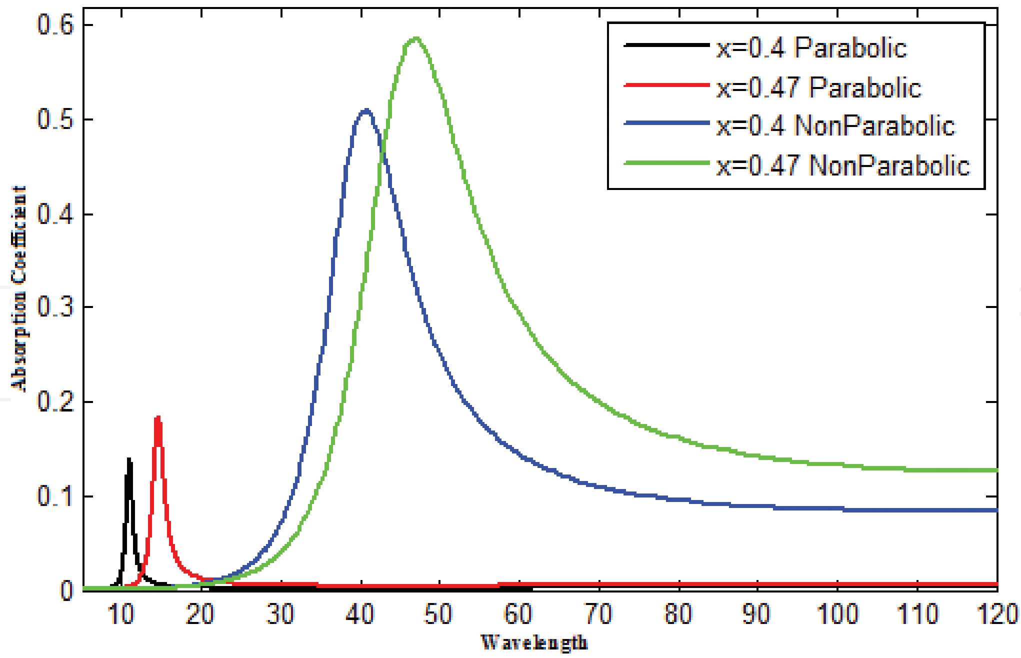

Figure 9. Absorption coefficient for different material composition with wavelength variation for nonparabolic and parabolic dispersion.

6. Band structure of quantum cascade laser

Electronic band structure of quantum cascade laser is analytically computed in presence of electric field applied along the direction of quantum confinement. At first, electronic and optoelectronic properties of the MQW structure is calculated. Next, miniband formation is observed for quantum cascade laser for a few precise magnitudes of electric fields. Separation of the miniband w.r.t. lowest energy band is calculated [68]. $Al_xGa_{1-x}As/GaAs$ composition is taken into account with the incorporation of Ben-Daniel Duke boundary conditions at hetero-interfaces. Eigenstates are calculated in presence and absence of Kane-type first-order conduction band nonparabolicity. Its variation as a function of applied field is determined, and is compared with the findings of zero bias conditions.

Figures 10–12 represent the electronic band structure of quantum cascade laser. For biasing, electric field is applied along the direction of quantum confinement, and eigenstates are computed. Results are also obtained when field is absent. While designing the structure, the most important aspect is that a distinguishable separation between injector and active region should be kept along with the miniband formation [68]. **Figure 10** shows the band diagram when external field is totally absent, and **Figure 11** demonstrated it for very high electric field (56.8×10^5 V/m). Here it may be noted that all the high magnitudes of electric field will not provide desirable QCL operation, as discrete miniband formation is necessary for that purpose. From the simulated observations, it may be indicated that the eigenenergy states are totally discrete in absence of external excitation, which are nothing but the eigenstates of a simple multiple quantum-well (MQW) structure.

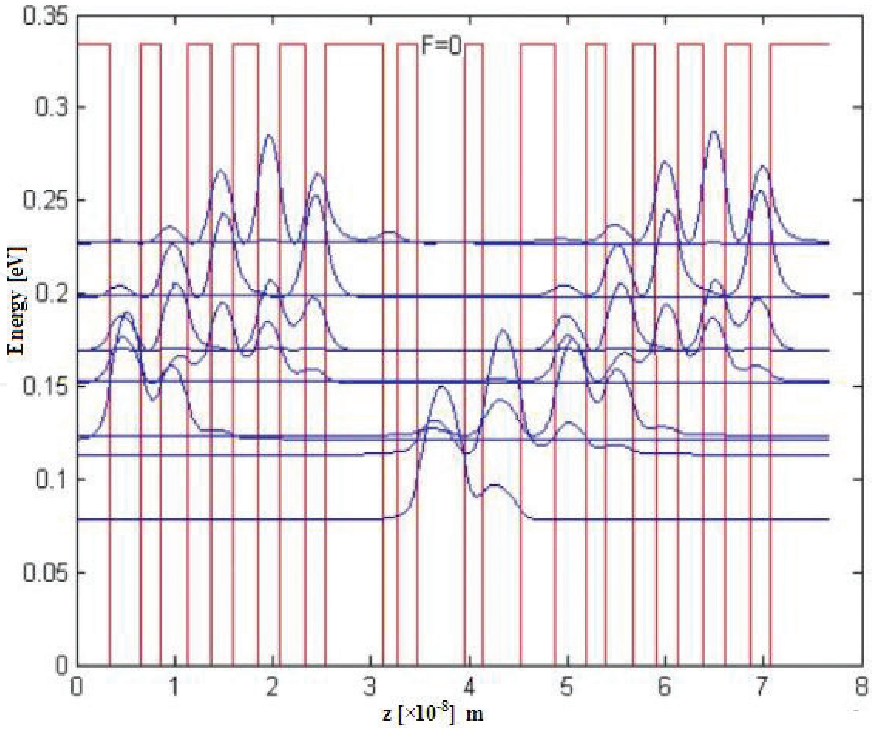

Figure 10. Electronic band structure of QCL without external bias.

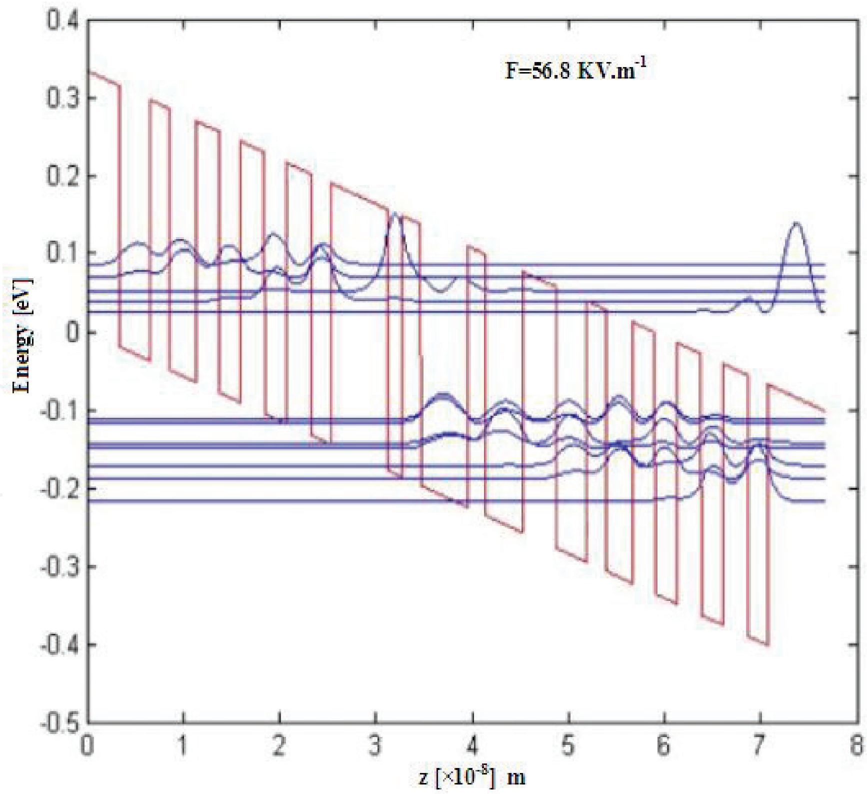

Figure 11. Electronic band structure of QCL with 56.8×10^5 V/m.

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From **Figure 11**, it is observed that after application of very high electric field, miniband is formed over the ground state energy band. In this context, it may be noted down that after the injector region, active region starts, and the wavefunction starts to produce minibands. The energy gap between miniband and ground state energy band is distinguishable, which ensures the QCL operation. In this context, it may be pointed out that the magnitude of external field is chosen based on the structural dimensions and the material composition taken for the simulation. The structure is titled compared to **Figure 10**, along the direction of electric bias. Thus, the periodic growth of wavefunction in the miniband appears outside the confinement region, that is, in the quasi-continuous region. This band structure modulation is absent if the field is moderate (35.8×10^5 V/m).

Further reduction of electric field makes position of the miniband almost inside the confinement region, that is, miniband position is below the quasi-continuous region. This is shown in **Figure 12**. Eigenenergy variation with the applied bias for the laser is shown in **Figure 13**. Simulation result suggests that with increase of applied field, eigenenergy increases monotonically, and the rate reduces once filed crosses the value 35×10^5 V/m. Thus, stimulated emission between the miniband and the ground state energy band is effectively controlled by external bias.

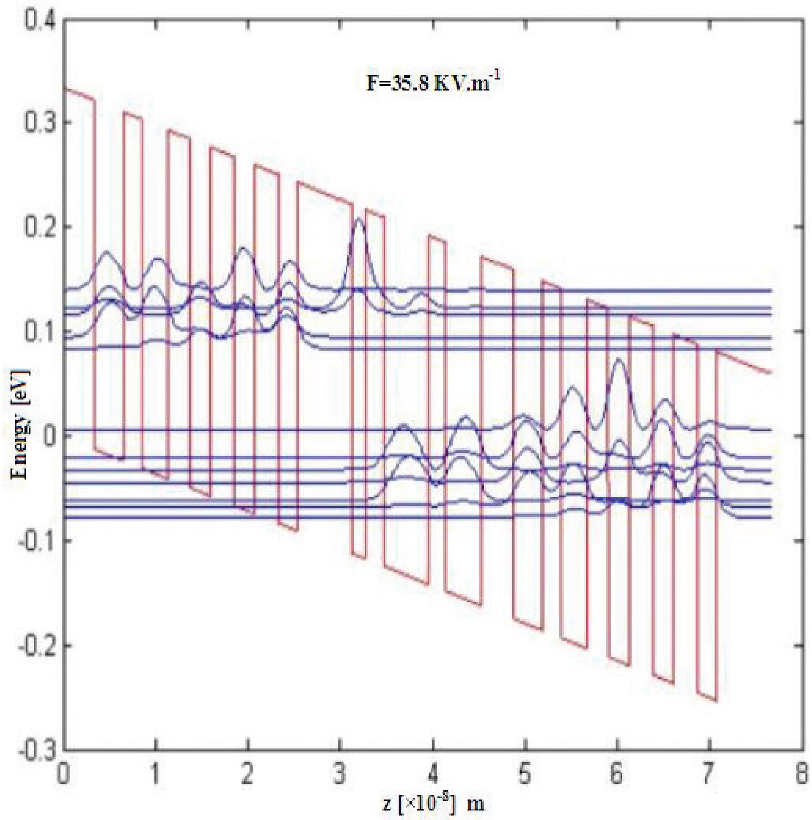

Figure 12. Electronic band structure of QCL with 35.8×10^5 V/m.

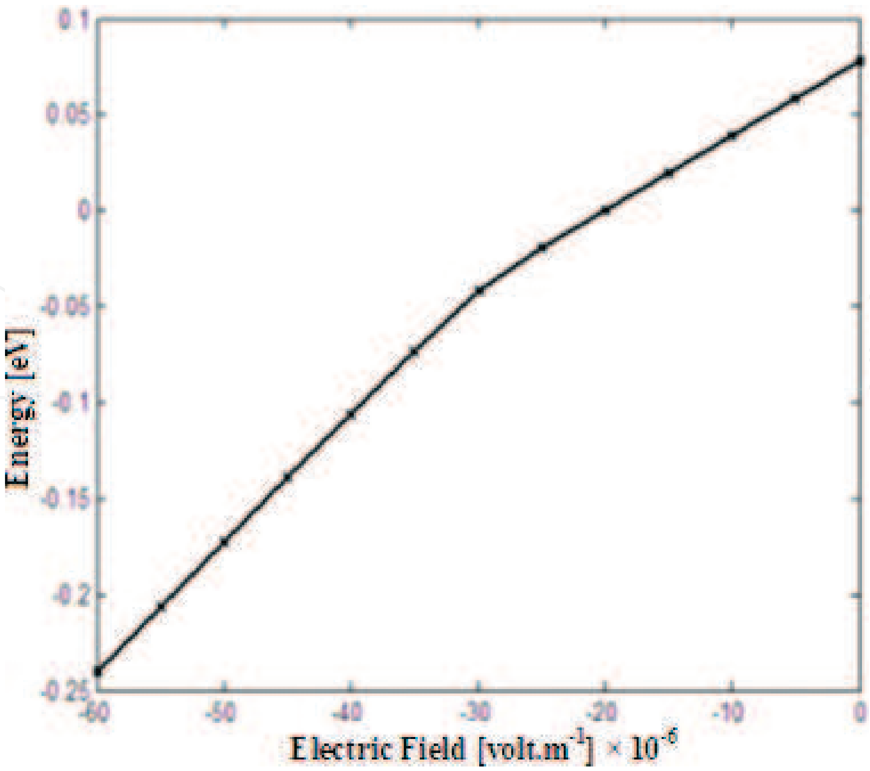

Figure 13. Variation of eigenenergy with applied field.

7. Conclusion

In this article, a detailed investigation on electrical and optoelectronic properties of multiple quantum well structure is carried out. Based on that structure, wavefunction in a quantum cascade laser at various biased conditions is analytically calculated and also for unbiased condition. It is proven and shown that miniband formation is only possible at some precise electric field. The method showed can also be applicable for the other structures. Key factor in this calculation is that position-dependent effective mass is considered for the simulation.

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