Electronic Band Structure of Quantum Cascade Laser

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Abstract Position of miniband and its separation w.r.t lowest energy band of a quantum cascade laser are analytically computed for different biasing conditions. Position-dependent effective mass following BenDaniel duke boundary conditions are considered in this simulation, which speaks in favour of realistic consideration. Findings are compared with that obtained under zero bias condition, and variation of eigenenergy of the lowest quantum state is computed as a function of electric field (applied along quantized direction). Length of the injector region is shown as a function of external bias. Result gives key information on electronic band structure of quantum cascade laser.

1 Introduction

Multiple quantum well structures are subject to theoretical and experimental research in last two decades because of the resonant tunnelling phenomenon [1], and novel photonic devices are already designed as transmitter [2] and receiver 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. Researchers have investigated the physics of resonant tunneling following the works of Esaki and Tsu [3], and series of theoretical [4] and experimental works [5] are reported thereafter. Theoretical

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researches are well supported by the advanced fabrication technologies [6], which allow tailoring the electronic and optoelectronic properties of quantum heterostructures. One such example is the THz laser design with low-dimensional semiconductor structures [7] with multiple layers, where miniband formation and its energy difference with lowest quantum energy state (lowermost energy band) plays crucial factor in governing the device performance [8] 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 [9]. 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 [10]. 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 is very important for theoretical researchers from the point of view of optoelectronic application.

In the present paper, band structure of quantum cascade laser is computed in presence of moderate and high electric field, and result is compared with zero field condition. Eigenenergy is determined for a range of bias. Comparative study is carried out with the energy obtained for nonparabolic dispersion relation.

2 Mathematical Modeling

With effective mass approximation, time-independent Schrödinger equation for electron wavefunction ψ is given by

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[\frac{1}{m^*(E,z)}\frac{d}{dz}\psi(z)\right] + V(z)\psi(z) - q\xi(z)\cdot z\cdot\psi(z) = E(z)\psi(z) \qquad (1)$$

where ζ(z) is the electric field applied along the direction of quantum confinement. Introducing finite difference technique, (1) can be modified as

$$\begin{aligned} -\frac{\hbar^2}{2}\left[\frac{1}{m^*(E,z)}\right]\left[\frac{\psi(z+1)+\psi(z-1)-2\psi(z)}{(\Delta z)^2}\right] \\ + V(z)\psi(z) - q\xi(z)\cdot z\cdot\psi(z) = E(z)\psi(z) \end{aligned} \qquad (2)$$

In order to introduce BenDaniel Duke boundary condition, we consider

$$\alpha = -\frac{\hbar^2}{(dz)^2[m^*(z)+m^*(z-dz)]} \qquad (3)$$

$$\beta = -\frac{\hbar^2}{(dz)^2[m^*(z) + m^*(z+dz)]} \tag{4}$$

We introduce diagonal and off-diagonal terms of the Hamiltonian matrix as

$$t_d = -\frac{\hbar^2}{(dz)^2[m^*(z) + m^*(z-dz)]} + V(z) - q\xi(z) \tag{5}$$

$$t_{off} = -\frac{\hbar^2}{(dz)^2[m^*(z) + m^*(z+dz)]} \tag{6}$$

where effective mass is taken as position dependent. After organizing the elements of the Hamiltonian, we use the equation

$$H\psi = E\psi \tag{7}$$

Solution of this equation gives the eigenstates of the structure with appropriate boundary conditions.

3 Results and Discussions

Figure 1 depicts the electronic band structure in absence and presence of external electric field in the quantum cascade laser. It may be mentioned in this context that layer dimensions is chosen in such a way that injector and active region separations may clearly be distinguished from the band diagram. The figure in left shows for zero bias, and figure in right exhibits for very high electric field (56.8 × 10^5 V/m). From the plot, it is seen that the energy states are discrete (as expected due to

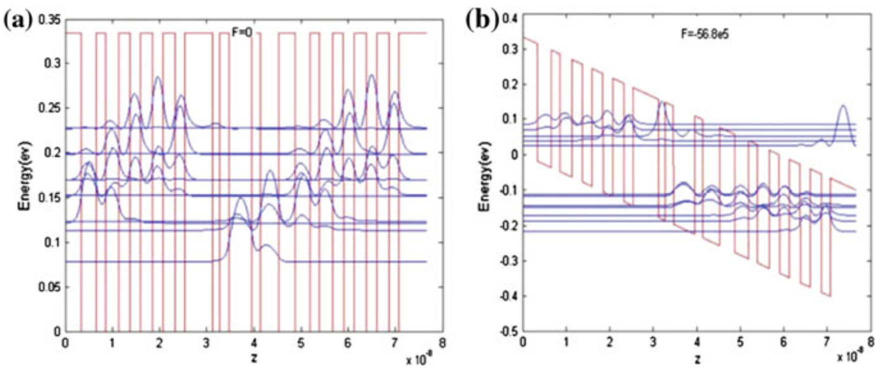

Fig. 1 **a** Band structure of QCL at unbiased condition. **b** Band structure of QCL at high bias

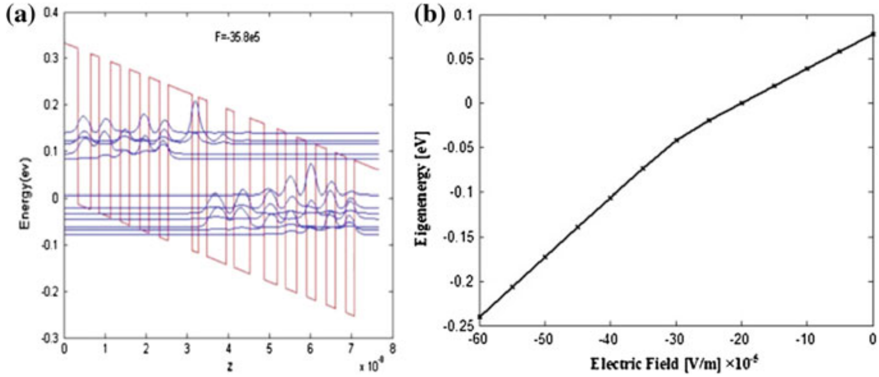

Fig. 2 **a** Band structure of QCL at moderate bias. **b** Eigenenergy variation of QCL with electric field

quantum confinement) in nature when field is not applied, which signifies the eigenstate of an otherwise multiple quantum well (MQW) structure. When strong electric field is applied, miniband is formed over the ground state energy band. It may be noted from the plot that after the injector region, the wavefunction starts to grow in the first miniband, which is the active region. Also due to the field, the structure is tilted, and thus the periodic growth of wavefuncion in the miniband appears outside the confinement region, i.e., in the quasi-continuous region. This modulation is absent if the field is moderate (35.8×10^5 V/m), which is represented in Fig. 2a (left). But moderate magnitude of electric field leads to the growth of wavefunction in the ground quantum state of the energy band. In this case, position of the miniband is found as almost inside the confinement region, i.e., miniband position is below the quasi-continuous region.

The right side of Fig. 2 shows the eigenenergy variation with the applied bias for the laser. The plot suggests that applied field is monotonically decreased with the increase of bias and the rate of increment increases when electric field is over 35×10^5 V/m. Thus stimulated emission between the miniband and the ground state energy band is effectively controlled by external bias.

4 Conclusion

The paper shows the wavefunction in a quantum cascade laser at various biased and unbiased conditions. Formation of miniband at some precise electric field is established. Result reveals that the miniband formation is very important for stimulated emission. 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, which is key for verification with experimental findings.

References

1. Davis, Kubis. T., Mehrotra. S. R., Klimeck. G., "Design concepts of terahertz quantum cascade lasers: Proposal for terahertz laser efficiency improvements", Applied Physics Letters, vol. 97, p. 261106 (2010).
2. Cooper. J. D., Valavanis. A., Ikonic. Z., Harrison. P., Cunningham. J. E., "Finite difference method for solving the Schrödinger equation with band nonparabolicity in mid-infrared quantum cascade lasers", Journal of Applied Physics, vol. 108, p. 113109 (2010).
3. Esaki. L, Tsu. R., "Superlattice and Negative Differential Conductivity in Semiconductors", IBM Journal of Research and Development, vol. 14(1), pp. 61–65 (1970).
4. Almansour. S. A., Hassen. D., "Theoretical Study of Electronic Transmission in Resonant Tunnelling Diodes based on GaAs/AlGaAs Double Barriers under Bias Voltage", Optics and Photonics Journal, vol. 4, pp. 39–45 (2014).
5. Toivonen. M., Jalonen. M., Pessa. M., Lefebvre. K. R., Anderson. N. G., "Experimental and theoretical studies of multi-quantum well structures for unipolar avalanche multiplication", Materials Science and Engineering: B, vol. 21(2–3), pp. 237–240 (1993).
6. Jogi. J., Verma. N., Gupta. M., Gupta. R. S., "Quantum Modeling of Electron Confinement in Double Triangular Quantum Well formed in Nanoscale Symmetric Double-Gate InAlAs/InGaAs/InP HEMT", International Semiconductor Device Research Symposium, pp. 1–2 (2011).
7. Razavipour. S. G., Dupont. E., Chan. C. W. I., Xu. C., Wasilewski. Z. R., Laframboise. S. R., Hu. Q., Ban. D., "A high carrier injection terahertz quantum cascade laser based on indirectly pumped scheme", Applied Physics Letters, vol. 104, p. 041111 (2014).
8. Hayata. H., Koshiba. M., Nakamura. K., Shimizu. A., "Eigenstate calculation of quantum well structures using finite elements", Electronics Letters, vol. 24, p. 614, 1988.
9. Bugajski. M., Kosiel. K., Szerling. A., Karbownik. P., Pierscinski. K., Pierscinska. D., Haldas. G., Kolek. A., "High performance GaAs/AlGaAs quantum cascade lasers: optimization of electrical and thermal properties", Proc. of SPIE, vol. 8432, p. 84320I (2012).