A Novel Band Structure Calculation for the Quantum Cascade Lasers with Conduction Band Nonparabolicity Effect

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Since the first demonstration in 1994[1], quantum cascade (QC) lasers have been developed as capable sources for mid-infrared to THz radiation. After decade's effort on the optimization of active region structures[2] and growth technology, QC lasers with high output power operating at room temperature in CW mode as well as pulsed mode have been achieved[3-4].

Since the operating wavelength of and the carrier dynamics in the QC lasers are determined mainly by a quantum well structure rather than bandgaps of materials, an accurate theoretical modeling is very important in the QC laser design. There have been various methods used to calculate the band profiles in the quantum well structures, which include the matrix approach[5], the transfer matrix method[6], and the finite difference method (FDM)[7]. The FDM is a quite straightforward method and advantageous in that all the subbands can be calculated simultaneously. However, this advantage of simultaneous calculation of all subbands hardly can be taken if the conduction band nonparabolicity effect[8] is included. Thus, in the previous work, to include the nonparabolicity effect, subbands were calculated sequentially and in each subband calculation, a good guess of an eigenenergy was to be made[9].

In this paper, we proposed the new band structure calculation method based on the FDM in which all subbands are calculated simultaneously even with taking into account the conduction band nonparabolicity effect. The key element of new approach is the using of the first Taylor's approximation of the position and energy dependency of the electron effective mass. With the proposed method, we can simultaneously calculate all the bound and quasi-bound energy levels, and corresponding wave functions for QC laser structures. The proposed method has been verified by being applied to calculate the conduction subband structures of the previously reported QC lasers[10-13]. The calculation results showed good agreement with the previously reported results. The figures below show the calculated subbands, and in the tables, our calculated energy values are compared to the previously reported values of measurement as well as the values of previous calculation.

References

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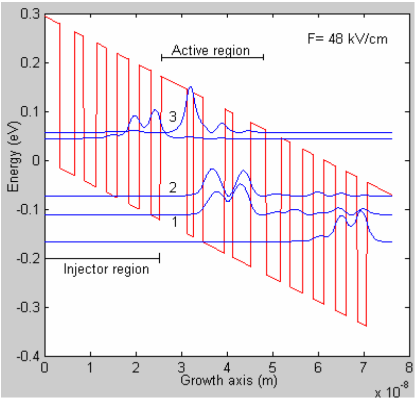

Fig. 1: Schematic illustration of conduction band diagram of a portion of the laser heterostructure at threshold bias, energy levels and relevant wave function (squared) for GaAs/ $Al_{0.33}Ga_{0.67}As$-based QC laser of Carlo Sirtori et al. [10].

Table 1

Comparison of transition energies in GaAs/ $Al_{0.33}Ga_{0.67}As$-based QC laser between experiment data, Sirtori's and our calculation

Transition energy	Sirtori's calculation	Our calculation	Experiment
ΔE_{21}	38 meV	38.2 meV	-
ΔE_{32}	134 mev	130.5 meV	131.6 meV

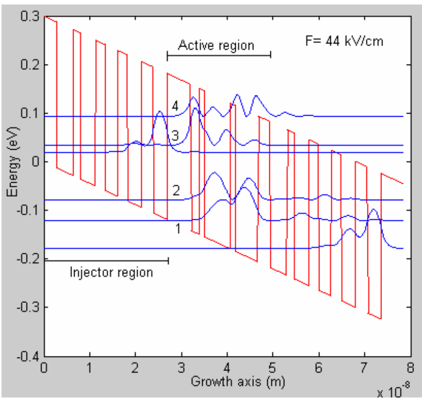

Fig. 2: Schematic illustration of conduction band diagram of a portion of the laser heterostructure at threshold bias, energy levels and relevant wave function (squared) for GaAs/ $Al_{0.33}Ga_{0.67}As$-based QC laser of P. Kruck et al. [11].

Table 2

Comparison of transition energies in the GaAs/ $Al_{0.33}Ga_{0.67}As$-based QC laser between Kruck's and our calculation

Transition energy	Kruck's calculation	Our calculation
ΔE_{32}	112 meV	112.0 meV
ΔE_{cont}	58 mev	59.4 meV

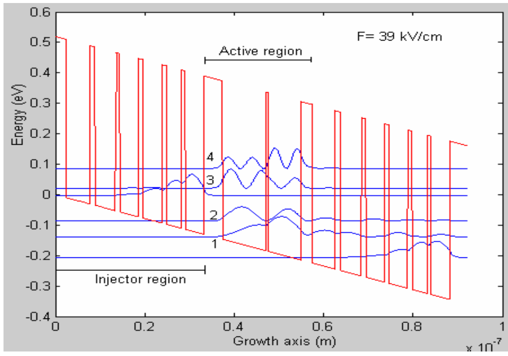

Fig. 3: Schematic illustration of the hetero-structure potential, energy levels, relevant wave function (squared) for $Al_{0.48}In_{0.52}As / Ga_{0.47}In_{0.53}As$ -based QC laser of Sirtori [12]. Sirtori's calculation of transition energy ΔE_{32} = 106.6 meV is in good agreement with our calculation (ΔE_{32} = 107.1 meV).

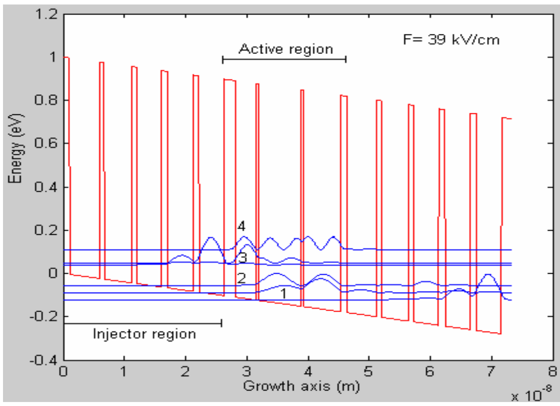

Fig. 4: Schematic illustration of conduction band profile of the laser heterostructure, energy levels, relevant wave function (squared) for AlAs/ GaAs -based QC laser of Becker [13]. Becker's calculation of transition energy ΔE_{32} = 109 meV is in good agreement with our calculation (ΔE_{32} = 105 meV).