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Influence of nonparabolicity on electronic structure of quantum cascade laser

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ABSTRACT

We analyze the influence of nonparabolicity on the bound electronic states in the conduction-band of quantum wells in external electric field. Numerical results, obtained by transfer matrix method are presented for active region of GaAs/$Al_{0.3}Ga_{0.7}As$ quantum cascade laser. The structure was initially optimized by genetic algorithm, using Kane's model of nonparabolicity, with emission wavelength set to $\lambda \approx 15.1$ μm. However, our numerical results indicate the change in lasing wavelength to 14.04 μm when using a more comprehensive description of nonparabolicity.

1. Introduction

When electrons occupy the energy levels on the order 100 meV above the bulk conduction-band edge of a semiconductor well material, nonparabolicity effects become significant. Several considerations of this problem can be found in the literature, introducing energy-dependent electron effective mass. First models which included nonparabolicity effects used a small number of bands, and treated the other bands as perturbations [1–4]. In [5,6] the authors used a more precise approach with higher conduction bands involved, in order to provide better description of conduction-band when energies are greater than 50 meV above the band edge. Starting from the method presented in [6] which assumes 14-band $k–p$ calculation, a more convenient method was developed, which used the bulk dispersion from [6] and from it determined the coefficients in an expansion of dispersion relation up to fourth order in wave vector [7–9]. It was stated in [9] that one possible boundary condition candidate to be used at the well/barrier interface is the one satisfying the conservation of probability current along the structure. This above mentioned boundary condition was derived in detail in [10] by double integration of Schrödinger equation. An exact approach for solving the Schrödinger equation in case of a semiconductor quantum well (QW) under applied bias is rather cumbersome, especially with nonparabolicity involved.

One of the numerous applications of a QW structure in the applied electric field is certainly quantum cascade laser (QCL). QCLs are powerful light sources for mid- and far-infrared spectral range which have turned out to be very efficient and reliable in free-space communications, medical diagnostics and chemical sensing [11–15]. Changing the design of the active region, one can obtain wide scope of operating wavelengths ranging from 3 μm up to 250 μm. Although the best performance in mid-infrared spectral range is achieved in GaInAs/AlInAs based QCLs [16,17], there are limitations concerning their chemical sensing applications [18]. On the other hand, GaAs/AlGaAs QCLs offer several benefits during fabrication since GaAs technology is well established and does not require extremely demanding growth process and precise control [19,20]. Band nonparabolicity parameters relevant for the effects considered in this work are well known, experimentally and theoretically, for GaAs/AlGaAs system, which is also lattice-matched to GaAs for any Al content. One needs to find optimal structure parameters for the desired wavelength using carefully selected optimization technique such as the genetic algorithm, which enables systematic search of the free parameters space and proves to be one of the best tools for global optimization problems [21–23]. In this paper we describe our model of quantum well in applied electric field and utilize it on a suitable QCL active region designed for the mid-infrared spectral range (15.1 μm). This active region was previously obtained by structural parameters optimization using genetic algorithm which assumes a simpler relation for nonparabolicity effects. Our numerical results show that the bound states energies become shifted within the improved model, and that the lasing wavelength actually amounts to 14.04 μm.

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2. Theoretical considerations

In case of a nanostructure, the Schrödinger equation for the envelope wave function $\psi(z)$ reads:

$$\hat{H}\psi(z) = \frac{d^2}{dz^2}\alpha_0(z)\frac{d^2\psi(z)}{dz^2} - \frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m^*(z)}\frac{d\psi(z)}{dz} + U(z)\psi(z) = E\psi(z), \quad (1)$$

where m^* is the effective mass at the bottom of the conduction-band, α_0 is the nonparabolicity parameter and $U(z)$ is potential energy. If the concentration of ionized impurities is not very high, we may assume that $U(z)$ originates from the conduction-band discontinuity only. The formula (1) is valid when the in-plane wave vector is equal to zero. Otherwise, additional terms depending on the components of in-plane wave vector should appear, as given in [9]. This form of the Schrödinger equation arises from a model which includes interaction of the lowest conduction band with the light-hole band, split-off band and higher conduction bands, as stated in [9]. A simpler model for electrons in the conduction-band, which considers only interaction between conduction and light-hole bands, yields Schrödinger equation valid at the bottom of the subbands, where the in-plane wave vector is zero [24]:

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[\frac{1}{M(z,E)}\frac{d\psi(z)}{dz}\right] + U(z)\psi(z) = E\psi(z). \quad (2)$$

Here $M(z,E)$ represents the effective mass in form:

$$M(z,E) = m^*(z)\left[1 + \frac{E - U(z)}{E_g(z)}\right], \quad (3)$$

where $E_g(z)$ signifies the spatial dependence of the direct energy gap.

The model presented in this paper uses the Schrödinger equation (1), and gives an improvement in the bound state energies compared to the second model which relies on Eq. (2).

Since the solutions of the Schrödinger equation are $\psi \sim e^{ikz}$, the dispersion relation in a single material (i.e. GaAs) reads:

$$\alpha_0 k^4 + \frac{\hbar^2 k^2}{2m^*} = E - U, \quad \alpha_0 < 0 \quad (4)$$

where U is the potential energy at the bottom of the material's conduction-band and we can set $U = 0$.

Algebraically, Eq. (4) has four solutions:

$$(k^2)_{1/2} = \frac{\hbar^2}{4|\alpha_0|m^*}\left[1 \pm \sqrt{1 - 16|\alpha_0|E\left(\frac{m^*}{\hbar^2}\right)^2}\right]. \quad (5)$$

However, when $E > 0$ and parameter α_0 approaches zero (the case of parabolic dispersion relation) it is obvious that a pair of solutions with + sign diverges, and thus does not possess physical justification. The only two solutions remaining are from the − branch:

$$k^2 = \frac{\hbar^2}{4|\alpha_0|m^*}\left[1 - \sqrt{1 - 16|\alpha_0|E\left(\frac{m^*}{\hbar^2}\right)^2}\right]. \quad (6)$$

Similarly, when $E < 0$, it can be shown that solutions are in the following format:

$$\kappa^2 = \frac{\hbar^2}{4|\alpha_0|m^*}\left[-1 + \sqrt{1 + 16|\alpha_0||E|\left(\frac{m^*}{\hbar^2}\right)^2}\right], \quad (7)$$

where $\kappa = \pm ik$. One can easily see from the first derivative of the dispersion relation that it has a minimum at $k = 0$ and maximum value of:

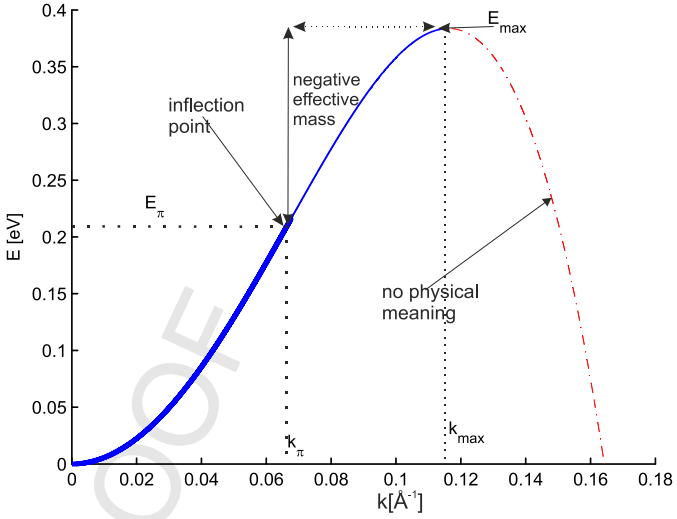

Fig. 1. Dispersion relation for $k > 0$. Note that for $k > k_{max}$ the branch does not have a physical meaning.

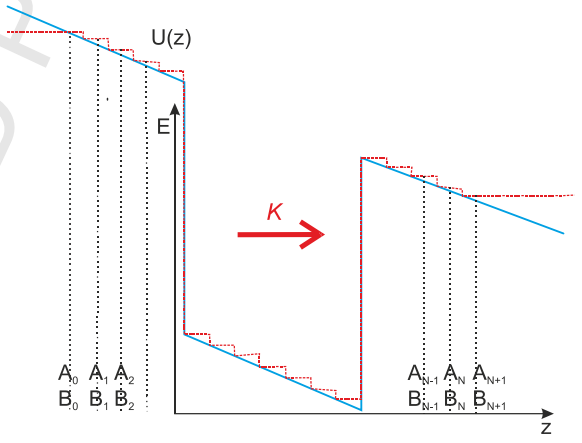

Fig. 2. In case when a moderate electric field is applied (i.e. $K = 45\ \mathrm{kV\,cm^{-1}}$), it is acceptable to approximate the potential at structure's ends with horizontal lines.

$$E_{max} = \frac{\hbar^4}{16|\alpha_0|(m^*)^2}, \quad \text{when } k_{max}^2 = \frac{\hbar^2}{4|\alpha_0|m^*}. \quad (8)$$

In case of GaAs, the maximum energy is $E_{max} = 384$ meV (Fig. 1). Inflection point of − branch of the dispersion relation lies at the energy $E_\pi = (5E_{max})/9$, which corresponds to 213 meV in GaAs. Starting from definition of the effective mass:

$$\frac{1}{m(k)} = \frac{1}{\hbar^2}\frac{d^2E(k)}{dk^2} = \frac{12\alpha_0 k^2}{\hbar^2} + \frac{1}{m^*}, \quad (9)$$

it is clear that for energies greater than E_π, effective mass in conduction-band becomes negative.

The application of electric field to the QW provides external adjustment of electronic structure and optical properties of the well, which can be utilized in numerous applications (i.e. realization of QCLs). The field alters the potential as shown in Fig. 2.

If we assume that the field exists in the entire range of z-coordinate from $-\infty$ to $+\infty$, strictly speaking, bound states do not exist anymore and the energy spectrum became continuous. However, in case of moderate external electric fields, the states that were previously bound, evolve into so-called quasi-bound states after the application of bias, which can then still be treated as bound under additional assumption that the potential is constant far enough from the well [25]. This consideration is exploited in our model in order to solve Eq. (1) in a simpler