Influence of thin AlAs layer insertion on intersubband optical transitions in GaAs/AlGaAs
quantum- well structures

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Abstract

In this work, we demonstrate the thin AlAs layer insertion into GaAs/AlGaAs quantum well (QW) structures and its influence in energy transition in the frequency range of mid-infrared. To realize the more accurate calculation, the graded interface model of QW structures is integrated into our self-consistent solving of Schrodinger and Poisson equations to obtain the energy level and envelope wave functions of QW. We find the thin AlAs layer inserted at various positions in the well can obviously tune intersubband optical transitions. The corresponding tuning range can be 50meV. We find that the thicker AlAs layer (2 monolayers) can provide wider tuning range and larger oscillator strength between subbands 1 and 3, compared with the thinner one (1 monolayer). Our results suggest that thin semiconductor layer may be an idea optimization design for the quantum well terahertz lasers which are based on optical pumping with mid-infrared lasers.

1. Introduction

Terahertz (THz) intersubband lasers, which can be realized by optically pumped [1-4] or electrically excited [5-6] quantum well structures, is based on intersubband (ISB) transitions between specific subbands within a multiple quantum well (QW) heterostructure. The typical designs of the active region for the optically pumped THz lasers are based on a three-level system [7-9]. For these designs the optical ISB absorption between the ground subband and the upper laser subband and the fast transition from the lower laser subband to the ground subband are two key points for the optimization of device performance.

Different from other semiconductor lasers, a THz intersubband laser is a unipolar laser and employs engineered transitions and energy levels within the conduction band of a complex QW. In recent years, several papers have been published about intersubband

transitions (ISBTs) in quantum wells (QW) with AlAs monolayer insertion. F. Castellano et al [10] measured mid-infrared intersubband absorption in InAs/AlSb QW systems with thin AlSb barriers. An AlAs submonolayer inserted into GaAs QWs was found to be a feasible method to tune the intersubband transition energy and linewidth [11]. The study [12] by the photoluminescence spectroscopy found that the electronic properties of the confined electrons is strongly influenced by a monolayer AlAs insertion in the modulation doped QW structures. All of the studies above were based on the abrupt interface models to calculate the energy levels and wavefunctions of QWs. However, N. Suzuki et al [13] found that the measured transition wavelengths for thinner wells were longer than the theoretical ones. This is thought to be due to the interface gradient of QWs. The graded interfaces in QWs were also verified by experimental results [14, 15] and further employed to improve the accurate calculations of electron sheet densities [16].

The AlAs monolayer not only can efficiently modify the intersubband transition between the ground state (subband 1) and the first excited state (subband 2), as indicated in [11], but also provides important features [12]: obviously change the electron-phonon scattering and effective mass of electrons. Considering these advantages, we in this paper try to investigate the possibility to introduce an AlAs monolayer to vary the intersubband transition between subband 1 and subband 3 in GaAs/AlGaAs QWs, to meet the mid-infrared intersubband absorption for the THz laser prototypes. We introduce the graded interface model into our calculations and further discuss the its difference with the abrupt interface.

2. Numerical Models

In the effective mass approximation, the energy levels and the corresponding wave functions for electrons in the GaAs/Al_xGa_{1-x}As QW are obtained by solving the Schrodinger and Poisson equations self-consistently using the finite element method [17]:

$$-\frac{\hbar^2}{2} \frac{d}{dz} \left(\frac{1}{m^*(z)} \frac{d}{dz} \right) \xi_i(z) + V(z) \xi_i(z) = E_i \xi_i(z) \quad (1)$$

$$\frac{d}{dz} \left(\epsilon_r(z) \frac{d}{dz} \right) \phi_e(z) = \frac{-e(N_d^+(z) - n(z))}{\epsilon_0} \quad (2)$$

where z is the space coordinate and parallels to the growth, m^* is the space dependent

electron effective mass, ε_0 is the dielectric constant in vacuum and $\varepsilon_r(z)$ is the relative dielectric constant, e is the free electron charge, $\hbar$ is the reduced Planck constant, E_i and ξ_i are energy eigenvalue and envelope wave function of the i th subband, respectively, $V(z)$ is the total potential energy, which is defined by

$$V(z) = -e\phi(z) + \Delta E_c(z) + V_{xc}(z) \quad (3)$$

where $\phi(z)$ is the Hartree potential due to the electrostatic interaction, and $\Delta E_c(z)$ is the conduction band-edge offset in the QW. The exchange-correlation potential $V_{xc}(z)$ can be formulated in an analytic form [18]

$$V_{xc}(z) = \frac{e^2}{4\pi^2 \varepsilon(z) a_B(z) r_s(z)} \left(\frac{9\pi}{4} \right)^{1/3} \left\{ 1 + 0.0545 r_s(z) \ln \left[1 + \frac{11.4}{r_s(z)} \right] \right\} \quad (4)$$

where $a_B = \varepsilon(z) \hbar^2 / e^2 m^*(z)$, $r_s(z) = \left\{ (3/4\pi) [a_B^3(z) N(z)]^{-1} \right\}^{1/3}$.

The position-dependent concentration of ionized impurities $N_d^+(z)$ in (2) is determined by

$$N_d^+(z) = \frac{N_d(z)}{1 + 2 \exp \left[\frac{E_f + E_d - V(z)}{k_B T} \right]} \quad (5)$$

By means of the density matrix method, the total optical absorption coefficient of the intersubband transitions can be expressed as a function of photon energy, which is proportional to $|M_{if}|^2$ [19], where M_{if} is the dipole matrix element,

$$M_{if} = \int_0^L \varphi_i(z) z \varphi_f(z) dz \quad (6)$$

For thinner wells, the measured transition wavelengths were longer than the theoretical ones, which was well explained by a model assuming 2- to 3- ML-thick interface graded layers [13]. Therefore, in this work, we use the graded interfacial profile shown in Fig. 1 to calculate the QW band structure, and thereby theoretically study the intersubband transition. Fig. 1 shows the electron potentials of GaAs/AlGaAs QW with an AlAs monolayer (0.26nm) inserted at the middle of QW well. The barrier layers are uniformly doped n type to yield an

electron sheet density n_s of $6.0 \times 10^{10} \text{ cm}^{-2}$. The temperature is assumed 293K. The subband wave functions indicated by dash and solid curves in Fig. 1 are calculated with the abrupt and graded interfacial profile, respectively. Fig. 1(a) is with the graded layer thickness 0.26nm (that is, one monolayer ML), and Fig. 1(b) is with the graded layer thickness 0.52nm (2ML). The graded interfacial model is found obviously amending the calculated energy levels and wavefunctions. The quantum well with 15nm can generate transition energy between subband 1 and 3 which actually is covered by the optical source provided by a CO₂ laser.

Fig. 1 The conduction band profiles in Al_xGa_{1-x}As/GaAs QW with an AlAs monolayer, and

the structural parameters. The three lines in the QW indicate the envelope functions of the first, second, and third subbands, respectively. (a) abrupt interface profile; (b) non-abrupt interface profile.

3. Results and Discussion

In this section, the calculation model described above is applied to design the QW structure for the mid-infrared intersubband absorption. Fig. 2 shows Intersubband transition energies as functions of the insertion position of the AlAs monolayer when the abrupt (dash-dot lines) and graded (solid) interfacial profiles are respectively used. The corresponding graded layer thickness (w_g) is assumed 1ML. Let us firstly look at the intersubband transition between subband 1 and subband 2, indicated by the circle symbols in Fig. 2. The corresponding transition energy increase and then decrease with increasing insertion position. This result is consistent with that obtained in Ref. 11. The square and triangle symbols in Fig. 2 are for the intersubband transitions between subband 1 and subband 3, and between subband 2 and 3, respectively. From them, we find that the transition energy first decrease and then increase with increasing the monolayer insertion position, which is quite different to that of transition energy between subband 1 and subband 2.

Fig. 2 Intersubband transition energies as functions of the insertion position of the AlAs monolayer (0.26nm). Dash-dot and solid lines are calculated from the abrupt and graded interfacial profiles, respectively. The graded layer thickness (w_g) is assumed 0.26nm. The

square symbol is for the transition between subband 1 and subband 3, the triangle symbol for the transition between subband 2 and subband 3, the circle symbol for the transition between subband 1 and subband 2.

The dash-dot and solid lines in Fig. 2 are calculated from the abrupt and graded interfacial profiles, respectively. There is a feature for the insertion position dependence of transition energy in Fig. 2: the graded interfacial profile gives rise to flatter variations with the insertion position, compared with the abrupt interfacial profile. For the comparison, we calculate the transition energy with different w_g , which is shown in Fig. 3. We find the graded interfacial profile has more influence in the upper levels, compared with the lower levels.

Fig. 3 Intersubband transition energies as functions of the insertion position of the AlAs monolayer with the graded interfacial profile used. Dash-dot and solid lines are calculated with the graded layer thickness (w_g) 1ML and 2ML, respectively. The symbols have the same meanings as in Fig. 2.

We use the graded interfacial QW and let $w_g = 2\text{ML}$, as shown in Fig. 1(b), and set w_b to be 1ML and 2ML, respectively. The corresponding calculated transition energy is compared in Fig. 4. We find that the tuned energy range is larger for 2ML AlAs barrier than for 1ML AlAs barrier. Among them, we can see that the tuned range for the transition between

subband 2 and 3 is the largest, which can be 50meV, shown by the triangle symbol-solid line in Fig.4.

Fig. 4 Intersubband transition energies as functions of the insertion position of the AlAs barrier with the graded interfacial profile used. Dash-dot and solid lines are calculated with the barrier thickness (w_b) 1ML and 2ML, respectively. The symbols have the same meanings as in Fig. 2.

The optical intersubband absorption is proportional to the dipole matrix element M_{if} , as expressed in Equ. (6). Fig. 5 (a) and (b) indicate the change of M_{12} and M_{13} with different insertion position of the AlAs barrier, from which we can find some important information. (1) for intersubband absorption between subbands 1 and 2, we obtain the maximum oscillator strength when the AlAs layer is inserted at 0.0nm, that is, the middle of the well, but for intersubband absorption between subbands 1 and 3, the maximum values occur at 2.0nm. M_{13} is very small when the AlAs layer is at 0.0nm. We know that when the AlAs layer is inserted at 0.0nm, the QW structure is symmetrical, so that the transition between subbands 1 and 3 is prohibited; (2) from M_{12} shown in Fig. 5(a), we find that if we move the AlAs layers away from the central position, the dipole matrix elements for $w_b = 1\text{ML}$ and $w_b = 2\text{ML}$ are both decrease, but the thinner AlAs layer gives rise to

relatively larger dipole matrix elements than the thicker one when the insertion position is over 1nm. For M_{13} , shown in Fig. 5(b), the result is contrary: The thicker AlAs layer with $w_b=0.52\text{nm}$ can result in larger dipole matrix elements.

Fig. 5 Dipole matrix element (a) M_{12} and (b) M_{13} as functions of the insertion position of the AlAs barrier with the graded interfacial profile used. Dash-dot and solid lines are calculated with $w_b = 1\text{ML}$ and 2ML , respectively.

4. Conclusion

We have numerically investigated the effect of a thin AlAs layer insertion into quantum well (QW) structures on the energy transition in the frequency range of mid-infrared. The graded interface model of QW structures is integrated into our self-consistent solving of Schrodinger and Poisson equations to obtain energy levels and envelope wave functions of QW, and is found that this model is necessary for the calculation of the upper levels of QW. On the other hands, it is found that the thin AlAs layer inserted at various positions in the well can obviously tune intersubband energy transitions. The corresponding tuning range can be 50meV. Our results also indicate that although the 1ML AlAs layer generally has advantage over the 2ML one in enhancing the dipole matrix elements between subbands 1 and 2, the 2ML AlAs layer can provide larger tuning range and larger oscillator strength between subbands 1 and 3 than the 1ML one. This work suggests that the thin semiconductor layer may be an idea optimization design for the quantum well terahertz lasers which are based on optical pumping with mid-infrared lasers.

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