Vol 18 No 9, September 2009
1674-1056/2009/18(09)/3905-04

Chinese Physics B

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Influence of applied electric field on the absorption coefficient and subband distances in asymmetrical AlN/GaN coupled double quantum wells*

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(Received 29 December 2008; revised manuscript received 7 April 2009)

The influence of applied electric fields on the absorption coefficient and subband distances in asymmetrical AlN/GaN coupled double quantum wells (CDQWs) has been investigated by solving Schrödinger and Poisson equations self-consistently. It is found that the absorption coefficient of the intersubband transition (ISBT) between the ground state and the third excited state ($1_{\rm odd}-2_{\rm even}$) can be equal to zero when the electric fields are applied in asymmetrical AlN/GaN CDQWs, which is related to applied electric fields induced symmetry recovery of these states. Meanwhile, the energy distances between $1_{\rm odd}-2_{\rm even}$ and $1_{\rm even}-2_{\rm even}$ subbands have different relationships from each other with the increase of applied electric fields due to the different polarization-induced potential drops between the left and the right wells. The results indicate that an electrical-optical modulator operated within the opto-communication wavelength range can be realized in spite of the strong polarization-induced electric fields in asymmetrical AlN/GaN CDQWs.

Keywords: AlN/GaN CDQWs, electrical–optical modulator, intersubband transition
PACC: 4280S, 7820J, 7830G

1. Introduction

GaN-based materials have attracted significant interest over the past few years owing to the possible applications in an ultraviolet photodetector, all-optical switches for optical communication networks, near-infrared photodetectors, and quantum cascade lasers.[1−7] The intersubband transitions (ISBTs) in $Al_xGa_{1-x}N$/GaN quantum wells (QWs) are shown to be advantageous over the other III–V semiconductor ones due to the large conduction band offset at $Al_xGa_{1-x}N$/GaN heterointerfaces, the large longitudinal-optical(LO)-phonon energy, and the large electron effective mass in GaN. These properties make the ISBTs in $Al_xGa_{1-x}N$/GaN QWs have a shorter wavelength and a shorter carrier relaxation time in comparison with those in other III–V semiconductor QWs,[8,9] which is beneficial to achieving ultrafast all-optical optoelectronic devices operating in an optical communication wavelength region.

Although the above-mentioned advantages of $Al_xGa_{1-x}N$/GaN CDQWs are useful to realize an electric-optical modulator operated within the opto-communication wavelength range, the strong polarization-induced electric fields lead to a potential drop between the left and the right wells, and thus result in Stark shift between the subbands in the two wells in spite of the same thickness and depth chosen for the two wells in $Al_xGa_{1-x}N$/GaN CDQWs.[10] It makes the two levels of the subband pair in $Al_xGa_{1-x}N$/GaN CDQWs be free of resonance, and thus the corresponding wavefunctions of the subband pair are mainly located in different wells of the CDQWs.[10] Therefore, it is not easy to obtain intersubband electric-optical modulation in symmetric $Al_xGa_{1-x}N$/GaN CDQWs. Nevou *et al*[7] and Cen *et al*[11] recently gave two schemes to modulate the ISBTs in AlN/GaN CDQWs. In these papers, the applied electric field is so big that the leak current of the modulator is big. In this letter, another

*Project supported by the National Natural Science Foundation of China (Grant Nos 60806042, 10774001, 60736033, 60890193 and 60628402), National Basic Research Program of China (Grant Nos 2006CB604908 and 2006CB921607), the Research Fund for the Doctoral Program of Higher Education in China (Grant Nos 200800011021 and 20060001018), and Beijing Natural Science Foundation (Grant No 4062017).
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modulation scheme of the ISBTs is given. The advantage of this scheme is that a smaller applied electric field is wanted to switch the modulator in spite of the strong polarization-induced electric fields in asymmetrical AlN/GaN CDQWs.

2. Theoretical calculation

The absorption coefficient of the ISBTs in the conduction band of AlN/GaN CDQWs can be expressed as a function of ω by the following formula[12]

$$\alpha(\omega) = \frac{\omega}{L}\sqrt{\frac{\mu_0}{\varepsilon_0\varepsilon_{\rm r}}}\sum_{m>n}\frac{|M_{mn}|^2\,[N_n - N_m](\hbar/\tau)}{[E_m - E_n - \hbar\omega]^2 + (\hbar/\tau)^2}, \tag{1}$$

where μ_0 is the permeability in a vacuum, ε_0 is the dielectric constant in a vacuum, $\varepsilon_{\rm r}$ is the relative dielectric constant, L is the total quantum well width, $\hbar$ is the reduced Planck constant, τ is the dephasing time, and M_{mn} is the dipole matrix. τ is assumed to be 20 fs in the calculation.[9]

M_{mn} is given by

$$M_{mn} = \int_{-L/2}^{L/2}\psi_m^*(z)ez\psi_n(z){\rm d}z, \tag{2}$$

where e is the electronic charge, N_i is the total electrons resided in the ith subband level, E_i and ψ_i $(i = m, n)$ are the energy level and the wavefunction of the ith subband, respectively. They are obtained by solving the Schrödinger and the Poisson equations self-consistently,

$$\begin{aligned}&-\frac{\hbar^2}{2}\frac{\rm d}{{\rm d}z}\left[\frac{1}{m^*(z)}\frac{\rm d}{{\rm d}z}\psi_i(z)\right]\\&+\left[V(z)+\frac{\Delta E_c}{e}+V_{xc}(z)-e\phi_{\rm H}(z)\right]\psi_i(z)\\&=E_i\psi_i(z),\end{aligned} \tag{3}$$

$$\begin{aligned}&\frac{\rm d}{{\rm d}z}\left[\varepsilon_0\varepsilon_{\rm r}\frac{\rm d}{{\rm d}z}\phi_{\rm H}(z)\right]\\&=-e\left[N_{\rm D}^+(z)-n_{\rm 2D}(z)-n_{\rm 3D}(z)+\delta(z)\Delta P\right],\end{aligned} \tag{4}$$

$$\begin{aligned}V_{\rm xc}(z) = -0.985\frac{e^2}{4\pi\varepsilon_0\varepsilon_{\rm r}}n^{1/3}(z)\Bigg\{1+\frac{0.034}{\alpha_{\rm H}^* n^{1/3}(z)}\\\times\ln\left[1+18.376a_{\rm H}^* n^{1/3}(z)\right]\Bigg\},\end{aligned} \tag{5}$$

where z is the space coordinate along the growth direction, $m^*(z)$ is the position-dependent effective mass, $V(z)$ the applied voltage, $\Delta E_{\rm c}$ is the conduction band offset, $\phi_{\rm H}(z)$ is the Hartree potential due to the electrostatic interaction, $V_{\rm xc}(z)$ is the exchange correlation potential,[13] $a_{\rm H}^* = 4\pi\varepsilon_0\varepsilon_{\rm r}\hbar^2/m^*(z)e^2$,[10] $\delta(z)$ is the Delta function, ΔP is the polarization field discontinuity at the heterointerface, $N_{\rm D}^+(z)$ is the ionized donor density, $n_{\rm 2D}(z)$ is the two dimensional (2D) electron density in all subbands, $n_{\rm 3D}(z)$ is the three dimensional (3D) electron density, and $n(z)$ is the sum of $n_{\rm 2D}(z)$ and $n_{\rm 3D}(z)$.

Under the equilibrium condition, $n_{\rm 2D}(z)$, $n_{\rm 3D}(z)$ and N_i are given by the formulas as follows, respectively.[10]

$$\begin{aligned}n_{\rm 2D}(z) &= \sum_i n_{{\rm 2D}_i}(z)\\&=\sum_i\frac{m^*kT}{\pi\hbar^2}\,|\psi_i(z)|^2\\&\quad\times\ln\left[1+\exp(\frac{E_{\rm F}-E_i}{kT})\right],\end{aligned} \tag{6}$$

$$n_{\rm 3D}(z) = N_{\rm c}(z)F_{1/2}\left(\frac{E_{\rm F}-E_i}{kT}\right), \tag{7}$$

$$N_i = \int n_{{\rm 2D}_i}(z){\rm d}z, \tag{8}$$

where k is the Boltzmann constant, T the absolute temperature, $E_{\rm F}$ the Fermi level, $N_{\rm c}(z)$ the 3D density of states and $F_{1/2}$ the Fermi-Dirac integral. In the calculation, the initial potential profile is assumed to be a rectangular potential profile. In order to ensure constringency of solving the Schrödinger and Poisson equations self-consistently, the potential profile of the next iteration is recalculated from a linear combination of new and old values of the potential profiles. The detailed self-consistent procedure can be found elsewhere.[14]

3. Results and discussion

In the calculation, the band gaps are chosen to be 3.4 eV for GaN and 6.2 eV for AlN, respectively.[10] The minimum of the conduction band profile of AlN/GaN CDQWs is defined as the zero reference energy. Under the assumption of the periodic potential model, the charge neutrality condition is adopted, which means that the sum of the charges in a periodic AlN/GaN CDQWs is zero. The structure of AlN/GaN CDQWs used in the calculation is 10 nm AlN/1.5 nm GaN/ 1 nm AlN/ 2.8 nm GaN. The total polarization field discontinuities (ΔP) are assumed as follows:[11]

$\Delta P_1 = 0.0168\mathrm{C/m}^2$, $\Delta P_2 = -0.0147\mathrm{C/m}^2$, $\Delta P_3 = -\Delta P_2$. The doping concentration in the left barrier is assumed to be $5 \times 10^{18}\mathrm{cm}^{-3}$. Dot L_1 is the reference energy, which is defined as zero. Electric fields are applied between dot A and dot B.

Figure 1 shows the schematic conduction band profile of asymmetrical AlN/GaN CDQWs and the moduli square of the wavefunctions under zero-applied electric fields. As shown in Fig.1, the polarization field induced potential drops lead to the asymmetry of the conduction band profile, and thus result in Stark shifts between the odd order and the even order subbands in the CDQWs. Due to the polarization-induced Stark shift, there is no resonance between the same subband levels in the two wells. This leads to the decrease of the tunneling probability of the electrons in the left and the right wells between each other. The wavefunctions of 1_{odd} and 2_{even} subbands are mainly located in the left well, and those of 1_{even}, 2_{odd} and 3_{odd} subbands are mainly located in the right one.

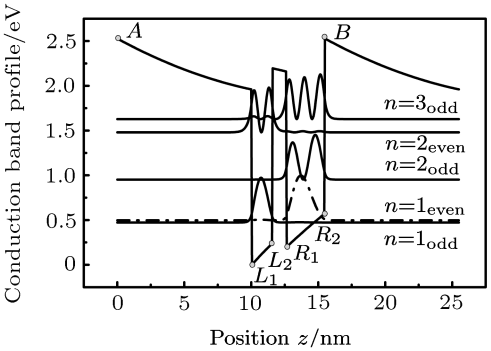


Fig.1. Schematic conduction band profile of AlN/GaN CDQWs and the moduli square of the wavefunctions under zero-applied electric fields.

Figure 2 shows the absorption coefficient of $1_{\mathrm{odd}} - 2_{\mathrm{even}}$ ISBT as a function of applied electric fields in AlN/GaN CDQWs. It is found that the absorption coefficient of $1_{\mathrm{odd}} - 2_{\mathrm{even}}$ ISBT is equal to zero when the applied electric field is equal to 280 kV/cm. The scheme in this letter gives a feasible approach to realize a modulator in spite of the strong polarization induced electric fields in AlN/GaN CDQWs. The zero-absorption coefficient of $1_{\mathrm{odd}} - 2_{\mathrm{even}}$ ISBT is not attributed to a reduced overlap of the final and initial states of the transition (Quantum Confined Stark Effect),[15] because it is equal to zero even if the overlap of the final and initial states of $1_{\mathrm{odd}} - 2_{\mathrm{even}}$ ISBT is reduced to zero by the applied electric field. This phenomenon can be explained as follows: AlN/GaN CDQWs can be considered as two isolated wells, defined as wells a and b, coupled by the central barrier. The wavefunctions of this system can be expanded in terms of the wavefunctions of the first two bound states $|\varphi_j\rangle$ $(j = 1, 2)$ of the two isolated wells. The dipole matrix element of $1_{\mathrm{odd}} - 2_{\mathrm{even}}$ ISBT in AlN/GaN CDQWs can be written as the sum of the contribution from the two wells a and b,

$$\langle 1_{\mathrm{odd}}|z|2_{\mathrm{even}}\rangle = \langle 1_{\mathrm{odd}}|\varphi_1^a\rangle\langle 2_{\mathrm{even}}|\varphi_2^a\rangle z_{12}^a + \langle 1_{\mathrm{odd}}|\varphi_1^b\rangle\langle 2_{\mathrm{even}}|\varphi_2^b\rangle z_{12}^b, \quad (9)$$

where z_{12}^a and z_{12}^b are the dipole matrix elements of the isolated wells. As $|1_{\mathrm{odd}}\rangle$ is the ground state of the coupled system, $\langle 1_{\mathrm{odd}}|\varphi_1^a\rangle$ and $\langle 1_{\mathrm{odd}}|\varphi_1^b\rangle$ have the same sign. However, since the third excited state $|2_{\mathrm{even}}\rangle$ crosses zero three and is constructed from the asymmetric wavefunctions $|\varphi_2^a\rangle$ and $|\varphi_2^b\rangle$, $\langle 2_{\mathrm{even}}|\varphi_2^a\rangle$ and $\langle 2_{\mathrm{even}}|\varphi_2^b\rangle$ have opposite signs. Therefore, corresponding to $1_{\mathrm{odd}} - 2_{\mathrm{even}}$ ISBT in AlN/GaN CDQWs, the two terms of (9) have opposite signs. When a large electric field is applied, the 1_{odd} and 2_{even} wavefunctions are mainly localized in the same well. As a result, only one term of (9) plays the dominant role and a large value of $\langle 1_{\mathrm{odd}}|z|2_{\mathrm{even}}\rangle$ is obtained. On the contrary, when some intermediate value of the electric field is applied, two terms of (9) play the role, which have opposite contributions to the transition. Then, a null is expected for the dipole matrix element $\langle 1_{\mathrm{odd}}|z|2_{\mathrm{even}}\rangle$.

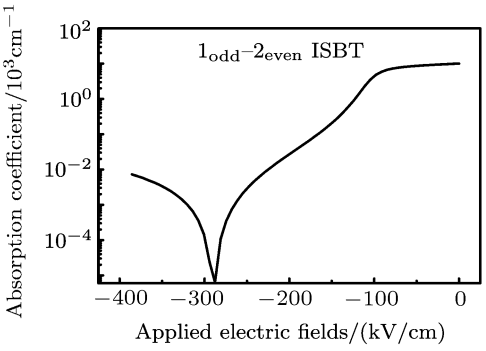


Fig.2. The absorption coefficient of $1_{\mathrm{odd}} - 2_{\mathrm{even}}$ ISBT as a function of the applied electric fields in AlN/GaN CDQWs.

Figure 3 shows (a) the different potential drops in the left and the right wells as a function of applied electric fields and (b) the energy distances of $1_{\mathrm{odd}} - 2_{\mathrm{even}}$ and $1_{\mathrm{even}} - 2_{\mathrm{even}}$ subbands as a function of applied electric fields, respectively. As shown in Fig.3(a), the potential drop in the left well (curve $L_2 - L_1$) is always smaller than that in the right one (curve $R_2 - R_1$) when applied electric fields increase.

It results in the subband energy levels in the left well having smaller shifts than those in the right one

with the increase of applied electric fields. As shown in Fig.3(b), the energy distance between the $1_{odd} - 2_{even}$ subband decreases, while the energy distance between the $1_{even} - 2_{even}$ subband increases, with the increase of applied electric fields. Such a phenomenon can be attributed to the different polarization-induced potential drops in the left and the right wells. When the applied electric field is zero, the 1_{odd} and 2_{even} wavefunctions are mainly located in the left well, while the 1_{even} wavefunctions are mainly located in the right one. The energy distance between the $1_{odd} - 2_{even}$ subbands decreases, while that between the $1_{even} - 2_{even}$ ones increases, with the increase of applied electric fields. However, when the applied electric field is large enough to change the 1_{odd} and 1_{even} wavefunctions between the left and right wells, the energy level shifts of the 1_{odd} and 2_{even} subbands are larger than the 1_{even} subband with the increase of applied electric fields. The subband energy distance between the $1_{even} - 2_{even}$ subbands decreases, while that between the $1_{odd} - 2_{even}$ ones increases, with the increase of applied electric fields.

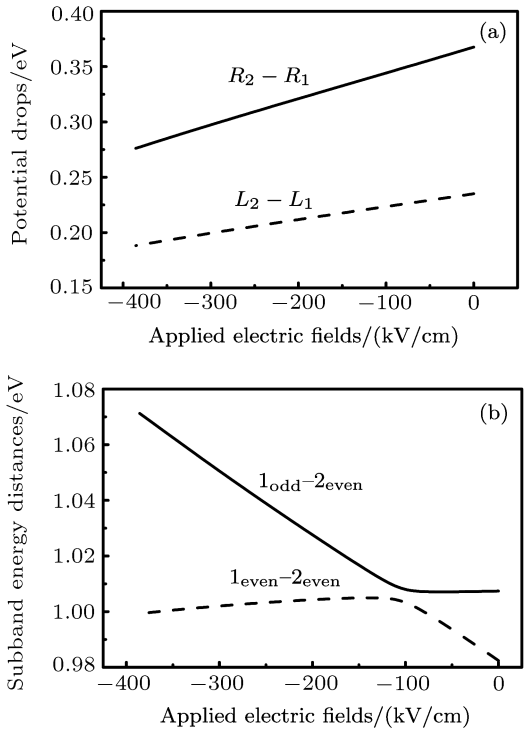


Fig.3. (a) Potential drops in the left and the right wells as a function of applied electric fields, and (b) the energy distances between 1_{odd}-2_{even} and 1_{even}-2_{even} subbands as a function of applied electric fields in AlN/GaN CDQWs.

4. Conclusions

The influence of applied electric fields on the absorption coefficient and subband distances in asymmetrical AlN/GaN CDQWs has been investigated by solving Schrödinger and Poisson equations self-consistently. It is found that the absorption coefficient of the $1_{odd} - 2_{even}$ ISBT can be equal to zero when the electric fields are applied in asymmetrical AlN/GaN CDQWs, which is related to applied electric fields induced symmetry recovery of these states. Meanwhile, the energy distances between $1_{odd} - 2_{even}$ and $1_{even} - 2_{even}$ subbands have different relationships from each other with the increase of applied electric fields due to the different polarization-induced potential drops between the left and the right wells. The results indicate that an electrical-optical modulator operated within the opto-communication wavelength range can be realized in spite of the strong polarization-induced electric fields in asymmetrical AlN/GaN CDQWs.

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