Influence of Polarization-Induced Electric Fields on Optical Properties of Intersubband Transitions in $Al_xGa_{1-x}N$/GaN Double Quantum Wells *

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Abstract: The influence of polarization-induced electric fields on the electron distribution and the optical properties of intersubband transitions (ISBT) in $Al_xGa_{1-x}N$/GaN coupled double quantum wells (DQWs) is investigated by self-consistent calculation. It is found that the polarization-induced potential drop leads to an asymmetric potential profile of $Al_xGa_{1-x}N$/GaN DQWs even though the two wells have the same width and depth. The polarization effects result in a very large Stark shift between the odd and even order subbands, thus shortening the wavelength of the ISBT between the first odd order and the second even order (1_{odd}-2_{even}) subbands. Meanwhile, the electron distribution becomes asymmetric due to the polarization effects, and the absorption coefficient of the 1_{odd}-2_{even} ISBT decreases with increasing polarization field discontinuity.

Key words: $Al_xGa_{1-x}N$/GaN DQWs; intersubband transition; polarization field discontinuity
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1 Introduction

Recently, intersubband transitions (ISBT) in nitride-based quantum wells (QWs) have attracted much attention because of their potential applications in optoelectronic devices, such as waveguide switches, infrared photodetectors, and quantum cascade lasers[1~3]. A large conduction band discontinuity on the order of 2eV for the AlN/GaN heterointerface, makes nitride-based QWs good candidates for devices operating in the near infrared range[4], especially at wavelengths of 1.3 and 1.55μm. A very short relaxation time, due to ultrafast carrier relaxation dynamics associated with the interaction between the electrons and LO-phonons[5,6], makes the optical switches good candidates for Tb/s optical time-division multiplexing[7].

In (0001)-oriented wurtzite nitride-based QWs, there exist very large polarization-induced electric fields that originate from piezoelectric and spontaneous polarization[8,9]. In symmetric $Al_xGa_{1-x}N$/GaN DQWs, in which the two wells have the same width and depth, the polarization-induced electric fields result in a potential drop between the two wells, resulting in a Stark shift between the subbands in the two wells. Therefore, the shorter wavelength of the ISBT in the DQWs is expected due to the polarization effects, which is beneficial for the realization of devices operating within the optical communication wavelength range. In this study, we have systematically studied the influence of the polarization-induced electric fields on the electron distribution, the wavelength, and the absorption coefficient of the ISBT in $Al_xGa_{1-x}N$/GaN DQWs. For greater accuracy, the exchange correlation potential is considered in

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the calculation.

2 Theoretical calculation

The linear optical absorption coefficient of the ISBT within the conduction band of $Al_x Ga_{1-x}N$/GaN DQWs can be given by[10]

$$\alpha(\omega) = \frac{\omega}{w}\sqrt{\frac{\mu_0}{\varepsilon_0\varepsilon}} \times \sum_m \sum_n |M_{mn}|^2 \frac{(N_n - N_m)(\hbar/\tau)}{(E_m - E_n - \hbar\omega)^2 + (\hbar/\tau)^2} \quad (1)$$

where μ_0 is the permeability in vacuum, ε_0 the dielectric constant in vacuum, ε the relative dielectric constant, w the total quantum well width, $\hbar$ the reduced Plank constant, τ the dephasing time, which is assumed to be 0.14ps in our calculation, and M_{mn} is the dipole matrix element, which is given by

$$M_{mn} = \int_{-w/2}^{w/2} \psi_m^*(z)|e|z\psi_n(z)\,dz \quad (2)$$

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

$$-\frac{\hbar^2}{2}\times\frac{d}{dz}\left(\frac{1}{m^*(z)}\times\frac{d}{dz}\psi_i(z)\right) + (V(z) + e\phi_H(z) + V_{xc}(z))\psi_i(z) = E_i\psi_i(z) \quad (3)$$

$$\frac{d}{dz}\left(\varepsilon_0\varepsilon\frac{d}{dz}\phi_H(z)\right) = -e(N_D^+(z) - n_{2D}(z) - n_{3D}(z)) \quad (4)$$

$$V_{xc}(z) = -0.985\frac{e^2}{4\pi\varepsilon_0\varepsilon}n^{1/3}(z) \times \left[1 + \frac{0.034}{a_B^* n^{1/3}(z)}\ln[1 + 18.376\,a_B^* n^{1/3}(z)]\right] \quad (5)$$

where z is the space coordinate in the growth direction, $m^*(z)$ the position-dependent effective mass[11], V(z) the bare well potential, which depends on the Al composition at the position z, $\phi_H(z)$ the Hartree term due to the electrostatic interaction, which is determined by the Poisson equation, $V_{xc}(z)$ the exchange correlation potential[12], $a_B^* = 4\pi\varepsilon_0\varepsilon\hbar^2/m^*e^2$, $N_D^+(z)$ the ionized donor density, $n_{2D}(z)$ the two dimensional (2D) electron density in all subbands, $n_{3D}(z)$ the three dimensional (3D) electron density, and n(z) is the sum of $n_{2D}(z)$ and $n_{3D}(z)$. Under the equilibrium condition, $n_{2D}(z)$, $n_{3D}(z)$, and N_i are given by

$$n_{2D}(z) = \sum n_{2D\_i}(z) = \sum \frac{m^* kT}{\pi\hbar^2}|\psi_i(z)|^2 \ln\left[1 + \exp\left(\frac{E_f - E_i}{kT}\right)\right] \quad (6)$$

$$n_{3D}(z) = N(z)\,F_{1/2}\left(\frac{E_f - E_i}{kT}\right) \quad (7)$$

$$N_i = \int n_{2D\_i}(z)\,dz \quad (8)$$

where k is the Boltzmann constant, T the absolute temperature, E_f the Fermi level, N(z) the 3D density of states, and $F_{1/2}$ the Fermi-Dirac integral.

In the calculation, the conduction band offset is assumed to be 70% of the total band offset[13]. The total polarization field discontinuity (ΔP) at the $Al_x Ga_{1-x}N$/GaN interface is included as a fitting parameter[14], and the relation between ΔP and the polarization-induced electric fields within the barrier and the well can be expressed as

$$F_{bb} = -\frac{(2\varepsilon_{cb} l_w + \varepsilon_w l_{cb})\Delta P_{bb} + \varepsilon_w l_{cb}\Delta P_{cb}}{\varepsilon_0(\varepsilon_w\varepsilon_{cb} l_{bb} + 2\varepsilon_{bb}\varepsilon_{cb} l_w + \varepsilon_{bb}\varepsilon_w l_{cb})} \quad (9)$$

$$F_w = \frac{\varepsilon_{cb} l_{bb}\Delta P_{bb} - \varepsilon_{bb} l_{cb}\Delta P_{cb}}{\varepsilon_0(\varepsilon_w\varepsilon_{cb} l_{bb} + 2\varepsilon_{bb}\varepsilon_{cb} l_w + \varepsilon_{bb}\varepsilon_w l_{cb})} \quad (10)$$

$$F_{cb} = \frac{(\varepsilon_w l_{bb} + 2\varepsilon_{bb} l_w)\Delta P_{cb} + \varepsilon_w l_{bb}\Delta P_{bb}}{\varepsilon_0(\varepsilon_w\varepsilon_{cb} l_{bb} + 2\varepsilon_{bb}\varepsilon_{cb} l_w + \varepsilon_{bb}\varepsilon_w l_{cb})} \quad (11)$$

where F_{bb} is the electric field in the bulk barriers, F_w the electric field in the wells, F_{cb} the electric field in the centric $Al_x Ga_{1-x}N$ barrier, ε_{bb} the dielectric constant of the bulk barrier, ε_w the dielectric constant of the well, ε_{cb} the dielectric constant of the centric $Al_x Ga_{1-x}N$ barrier, l_{bb} (= 10nm) the thickness of the bulk barrier, l_w (= 2nm) the thickness of the well, l_{cb} the thickness of the centric $Al_x Ga_{1-x}N$ barrier, ΔP_{bb} the polarization field discontinuity at the interface between the well and the bulk barrier, and ΔP_{cb} the polarization field discontinuity at the interface between the centric $Al_x Ga_{1-x}N$ barrier and the well.

3 Results and discussion

The $Al_x Ga_{1-x}N$/GaN DQW structure used in the calculation is 10nm $Al_{0.75}Ga_{0.25}N$/2.0nm GaN/1.0nm $Al_{0.70}Ga_{0.30}N$/2.0nm GaN/10nm $Al_{0.75}Ga_{0.25}N$. Figure 1 presents a schematic conduction band profile of the $Al_{0.75}Ga_{0.25}N$/GaN DQWs and the moduli squared of the wave functions. ΔP_{bb} and ΔP_{cb} are chosen to be 1.08×10^{-6} and 1.00×10^{-6} C/cm^2, respectively. The doping

concentration in the $Al_xGa_{1-x}N$ barriers is assumed to be $5.0 \times 10^{18}\ cm^{-3}$. Dot A is the reference energy, which is defined as 0. We find that $Al_xGa_{1-x}N$/GaN DQWs have an asymmetric conduction band profile although the width of the two wells and the conduction band offset at each interface are the same, and that the envelope wave functions of the odd and even order subbands are mainly located in the left and the right wells, respectively.

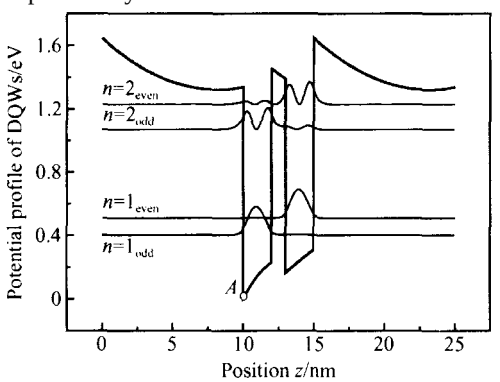

Fig. 1　Conduction band profile of $Al_xGa_{1-x}N$/GaN DQWs and the moduli squared of the wave functions

Polarization-induced electric fields in the wells and the barriers lead to a potential drop by the amount of $\sum eF_i l_i$, where e is the electron charge, F the polarization-induced electric field, l the thickness of the well layer or the barrier layer, and the subscript i = bb, w, and cb. As shown in Fig. 1, besides making the conduction band profile of $Al_xGa_{1-x}N$/GaN DQWs asymmetric, the polarization-induced potential drop also results in Stark shifts between the odd and even order subbands in $Al_xGa_{1-x}N$/GaN DQWs. Because of the polarization-induced Stark shifts there is no resonance between corresponding subband levels in the two wells, leading to a decrease in the tunnelling of the envelope wave functions between the left and right wells. Therefore, the wave functions of the odd and even order subbands are mainly located in the left and the right wells, respectively.

The electron densities distributed in the two wells for various ΔP between 0 and $1.44 \times 10^{-6}\ C/cm^2$ are shown in Fig. 2. When ΔP is non-zero, the electron densities distributed in the two wells are asymmetric. With increasing ΔP the electron density in the left well increases, while that in the right well decreases. The position of the electron distribution peak shifts to the left-hand-side in both wells.

Electron density decreases exponentially with increasing energy separation between the subband and the Fermi level (i.e. $E_i - E_f$). Therefore, the electrons in the DQWs reside mainly in the first subband levels, and there are more electrons in the 1_{odd} subband level than in the 1_{even} subband level. With increasing ΔP the energy separation between the 1_{even} subband and the Fermi level increases, while the energy separation between the 1_{odd} subband and the Fermi level decreases. This leads to the asymmetric electron distribution in the $Al_xGa_{1-x}N$/GaN DQWs. The electron density in the left well increases, while that in the right well decreases. Ahn et al. demonstrated that in an electric field the wave functions in the well were pushed to one side of the quantum well, and the ground wave function was pushed to the side with a lower potential. Thus, the position of the electron distribution peak shifts to the left-hand-side in both wells.

Figure 3 shows the absorption coefficients as functions of wavelength when ΔP_{bb} is equal to 0 and $7.2 \times 10^{-7}\ C/cm^2$, respectively, for $Al_xGa_{1-x}N$/GaN DQWs. Inset are the conduction band profile and the wave functions of the electrons in the DQWs for zero-polarization field discontinuity. When ΔP_{bb} is 0, there are two absorption peaks, and the absorption peaks of the transition between the first odd and the second even (1_{odd}-2_{even} transition) and the 1_{even}-2_{odd} transition are dominant. When ΔP_{bb} is not zero, there are four absorption peaks of the ISBT between the first and second subbands.

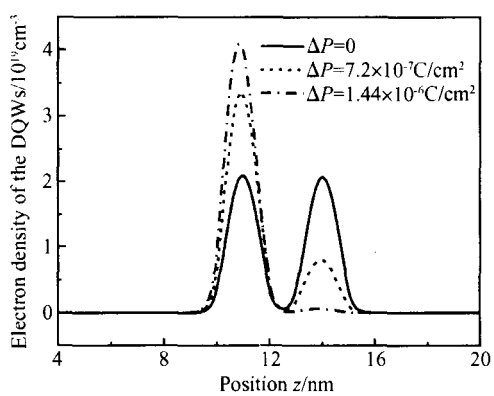

Fig. 2　Electron distribution in the two wells for various polarization field discontinuities ΔP between 0 and $1.44 \times 10^{-6}\ C/cm^2$

From Eq. (2), if $\psi_m(z)$ and $\psi_n(z)$ are similarly symmetrical, the dipole matrix element e-

quals 0. Therefore, the ISBT between the m-th and n-th subband levels is forbidden. If $\psi_m(z)$ and $\psi_n(z)$ have opposite symmetry or they are asymmetrical, the ISBT between the m-th and the n-th subband levels is allowed. As shown in the inset of Fig. 2, when ΔP_{bb} equals 0, the wave functions of the odd order subbands can be approximated as the even functions, while those of the even order subbands can be approximated as the odd functions. Therefore, the 1_{odd}-2_{odd} and the 1_{even}-2_{even} transitions are forbidden, while the 1_{odd}-2_{even} and the 1_{even}-2_{odd} transitions are allowed, and thus there are only two absorption peaks of the ISBT. As shown in Fig. 1, when ΔP_{bb} is not zero, all the moduli squared of the wave functions are asymmetrical due to the polarization-induced Stark shifts. Therefore, all the transitions between the first and second subbands are allowed, and thus there are four absorption peaks of the ISBT.

Figure 4 shows the influence of ΔP_{bb} on the wavelength and the absorption coefficient of the ISBT. The wavelength of the 1_{odd}-2_{even} ISBT decreases with increasing ΔP_{bb}, while that of the 1_{even}-2_{odd} ISBT increases with increasing ΔP_{bb}. The absorption coefficients of the 1_{odd}-2_{even} and the 1_{even}-2_{odd} transitions decrease with increasing ΔP_{bb}, while those of the 1_{odd}-2_{odd} and the 1_{even}-2_{even} transitions increase with increasing ΔP_{bb}. When ΔP_{bb} is larger than 5×10^{-7} C/cm^2, the absorption coefficient of the 1_{even}-2_{even} transition decreases with increasing ΔP_{bb}.

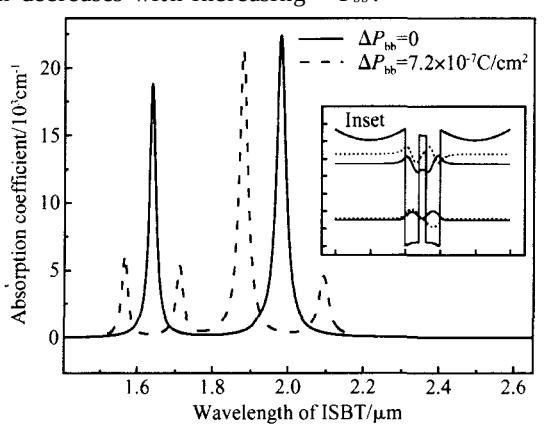

Fig. 3 Absorption coefficient of the ISBT between the first and second subbands as a function of the wavelength for zero and non-zero polarization field discontinuities in $Al_xGa_{1-x}N$/GaN DQWs Inset: the conduction band profile and the wave functions of the DQW for zero-polarization field discontinuity.

As we know, the electron densities are proportional to the moduli squared of the wave functions. Assuming that the electrons in each subband level are located at the peak position of the corresponding wave function, the Stark shifts between the odd order and the even order subband levels can be approximated as the potential drop between the left and the right wells. Therefore, the wavelength of the 1_{odd}-2_{even} ISBT decreases with increasing ΔP_{bb}, while that of the 1_{even}-2_{odd} ISBT increases with increasing ΔP_{bb}. On the other hand, the wave functions of the first odd order (1_{odd}) and the 2_{odd} subband levels shift to the left well with increasing ΔP_{bb}, while the 1_{even} and the 2_{even} wave functions shift to the right well with increasing ΔP_{bb}. The overlaps of wave functions of the odd order and the even order subbands decrease with increasing ΔP_{bb}, while those of two odd order subbands, as well as two even order subbands increase with increasing ΔP_{bb}. Therefore, the absorption coefficients of the 1_{odd}-2_{even} and the 1_{even}-2_{odd} ISBTs decrease with increasing ΔP_{bb}, while those of the 1_{odd}-2_{odd} and the 1_{even}-2_{even} ISBTs

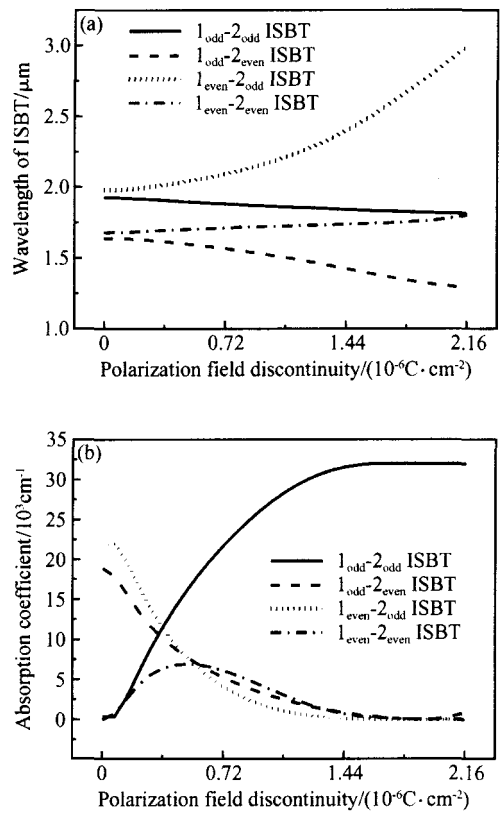

Fig. 4 Wavelength (a) and absorption coefficient (b) of the ISBT in $Al_xGa_{1-x}N$/GaN DQWs as functions of the polarization field discontinuity ΔP_{bb}

increase with increasing ΔP_{bb}. When ΔP_{bb} is larger than 5×10^{-7} C/cm^2, the absorption coefficient of the 1_{even}-2_{even} ISBT decreases with increasing ΔP_{bb} because the electrons at the 1_{even} subband decrease significantly with increasing ΔP_{bb} according to the Fermi-Dirac distribution.

4 Conclusion

The influence of the polarization-induced electric fields on the electron distribution and the optical properties of ISBT in $Al_xGa_{1-x}N$/GaN DQWs has been investigated by solving the Schrödinger and the Poisson equations self-consistently. It is found that the polarization-induced potential drop leads to an asymmetric potential profile of $Al_xGa_{1-x}N$/GaN DQWs even though the two wells have the same width and depth. The polarization effects result in a very large Stark shift between the odd and even order subbands, thus shortening the wavelength of the 1_{odd}-2_{even} ISBT. Meanwhile, the electron distribution becomes asymmetric due to the polarization effects, and the absorption coefficient of the 1_{odd}-2_{even} ISBT decreases with increasing polarization field discontinuity.

References

[1] Gmachl C, Ng H M, Cho A Y. Intersubband absorption in degenerately doped GaN/$Al_xGa_{1-x}N$ coupled double quantum wells. Appl Phys Lett, 2001, 79: 1590

[2] Gmachl C, Ng H M, Chu S GN G. Intersubband absorption at $\lambda \sim 1.55\mu$m in well- and modulation-doped GaN/AlGaN multiple quantum wells with superlattice barriers. Appl Phys Lett, 2000, 77: 3722

[3] Ishida A, Ose T, Nagasawa H, et al. Quantum-cascade structure in AlN/GaN system assisted by piezo-electric effect. Jpn J Appl Phys, 2002, 41: L236

[4] Iizuka N, Kaneko K, Suzuki N, et al. Ultrafast intersubband relaxation (150fs) in AlGaN/GaN multiple quantum wells. Appl Phys Lett, 2000, 77: 648

[5] Othonos A. Probing ultrafast carrier and phonon dynamics in semiconductors. J Appl Phys, 1998, 83: 1789

[6] Rudin S, Reineche T L. Electron-LO-phonon scattering rates in semiconductor quantum wells. Phys Rev B, 1990, 41: 7713

[7] Gmachl C, Ng H M, Cho A Y. Intersubband absorption in GaN/AlGaN multiple quantum wells in the wavelength range of $\lambda \sim 1.75$ - 4.2μm. Appl Phys Lett, 2000, 77: 334

[8] Ambacher O, Smart J, Shealy J R, et al. Two-dimensional electron gases induced by spontaneous and piezoelectric polarization charges in N- and Ga-face AlGaN/GaN heterostructures. J Appl Phys, 1999, 85: 3222

[9] Zhang Y F, Smorchkova Y, Elsass C, et al. Polarization effects and transport in AlGaN/GaN system. J Vac Sci Technol B, 2000, 18: 2322

[10] Huang Y, Lien C. Very large Stark shift in three-coupled-quantum wells and their application to tunable far-infrared photodetectors. J Appl Phys, 1995, 77: 3433

[11] De Paiva R, Alves J L A, Nogueira R A, et al. Theoretical study of the $Al_xGa_{1-x}N$ alloys. Mater Sci Eng B, 2002, 93: 2

[12] Brey L, Dempsey J, Johnson N F, et al. Infrared optical absorption in imperfect parabolic quantum wells. Phys Rev B, 1990, 42: 1240

[13] Ambacher O, Foutz B, Smart J, et al. Two dimensional electron gases induced by spontaneous and piezoelectric polarization in undoped and doped AlGaN/GaN heterostructures. J Appl Phys, 2000, 87: 334

[14] Garridoa J A, Sánchez-Rojas J L, Jiménez A, et al. Polarization fields determination in AlGaN/GaN heterostructure field-effect transistors from charge control analysis. Appl Phys Lett, 1999, 75: 2407

极化电场对 $Al_xGa_{1-x}N/GaN$ 双量子阱中子带间跃迁的光学性质的影响*

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摘要: 用自洽计算的方法研究了极化电场对 $Al_xGa_{1-x}N/GaN$ 双量子阱中子带间跃迁的光学性质和电子分布的影响. 发现极化场会导致电压降的出现,从而使得结构对称的 $Al_xGa_{1-x}N/GaN$ 双量子阱具有不对称的导带和价带. 极化效应还会使奇数序和偶数序的子带之间发生很大的 Stark 平移,从而使第一奇数序和第二偶数序子带之间的跃迁波长变短,这将有利于实现工作在通信窗口的光电子器件. 同时,由于导带分布的不对称性,电子分布也不对称,从而会影响吸收系数.

关键词: $Al_xGa_{1-x}N/GaN$ 双量子阱; 子带间跃迁; 极化场不连续

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