Intersubband transitions in $Al_{0.82}In_{0.18}N$/GaN single quantum well*

Wang Yu-Zhou(王宇宙), Li Ding(李 丁), Li Lei(李 磊), Liu Ning-Yang(刘宁炀), Liu Lei(刘 磊), Cao Wen-Yu(曹文彧), Chen Wei-Hua(陈伟华), and Hu Xiao-Dong(胡晓东)†

State Key Laboratory of Artificial Microstructure and Mesoscopic Physics, School of Physics, Peking University, Beijing 100871, *China*

(Received 6 September 2010; revised manuscript received 19 April 2011)

The influence of the width of a lattice-matched $Al_{0.82}In_{0.18}N$/GaN single quantum well (SQW) on the absorption coefficients and wavelength of the intersubband transition (ISBT) has been investigated by solving the Schrödinger and Poisson equations self-consistently. The wavelength of 1–2 ISBT increases with L, the thickness of the single quantum well, ranging from 2.88 μm to 3.59 μm. The absorption coefficients of 1–2 ISBT increase with L at first and then decrease with L, with a maximum when L is equal to 2.6 nm. The wavelength of 1–3 ISBT decreases with L at first and then increases with L, with a minimum when L is equal to 4 nm, ranging from approximately 2.03 μm to near 2.11 μm. The absorption coefficients of 1–3 ISBT decrease with L. The results indicate that mid-infrared can be realized by the $Al_{0.82}In_{0.18}N$/GaN SQW. In addition, the wavelength and absorption coefficients of ISBT can be adjusted by changing the width of the SQW.

Keywords: $Al_{0.82}In_{0.18}N$/GaN single quantum well, optoelectronic devices, mid-infrared, intersubband transition

PACS: 42.55.Px, 78.30.Fs, 42.70.Km, 68.65.Fg **DOI:** 10.1088/1674-1056/20/9/094207

1. Introduction

Extensive research has been focused on the intersubband transition (ISBT) in semiconductor quantum wells in recent years owing to their possible application in ultrafast optoelectronic devices, such as all-optical switches for optical communication networks, mid-infrared photodetectors and quantum cascade lasers.[1−7] The conduction band offset (CBO) between GaN and Al-containing alloys can exceed 1 eV, thus the intersubband energy is located in the near-infrared range.[8,9] For example, intersubband absorption at wavelengths as short as 1.08 μm from AlN/GaN quantum wells grown by molecular-beam epitaxy has been reported.[10] However, research progress has been hampered by difficulties related to the structural quality of the materials. Most of the intersubband studies reported in the literature employ high Al-content AlGaN or AlN alloys. There exists a large lattice mismatch between AlN or AlGaN and GaN, which results in the formation of cracks and/or dislocations. To overcome this problem, the straightforward solution would be to find materials with roughly the same lattice parameters. Fortunately, $Al_{1-x}In_xN$ alloy with indium content close to 18% is lattice-matched to GaN and the CBO of this system may be high enough for designing heterostructures with ISBT in the mid-infrared range.[11] In this article, we investigate the intersubband absorption in a lattice-matched AlInN/GaN single quantum well (SQW) theoretically. The large CBO and lack of a piezoelectric effect in the lattice-matched AlInN/GaN system make it an ideal alternative to traditional AlGaN/GaN or AlN/GaN systems.

We try to investigate the absorption coefficients and wavelength of the ISBT of the $Al_{0.82}In_{0.18}N$/GaN SQW. One method is to apply an external electric field normal to the quantum well layer and the other is to vary the width of the SQW. In this study, the influence of the width of the quantum well on the absorption coefficients and the wavelength of the ISBT in a single $Al_{0.82}In_{0.18}N$/GaN well has been studied by solving the Schrödinger and Poisson equations self-consistently.

*Project supported by the National High Technology Research and Development Program of China (Grant No. 2007AA03Z403), the National Natural Science Foundation of China (Grant Nos. 61076013 and 60776042), and the National Basic Research Program of China (Grant No. 2006CB921607).

†Corresponding author. E-mail: huxd@pku.edu.cn

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2. Theoretical calculation

The optical absorption coefficients of the ISBT in $Al_{0.82}In_{0.18}N$/GaN SQW can be expressed as a function of ω by the following formula:[12]

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

where μ_0 is the permeability in vacuum, ε_0 is the dielectric constant in vacuum, ε_r is the relative dielectric constant, L_t is the total quantum well width, $\hbar$ is the reduced Planck constant, N_i is the total amount of electrons residing in the ith subband level, E_i $(i = m, n)$ is the energy level of the ith subband, τ is the dephasing time and M_{mn} is the dipole matrix; τ is assumed to be 0.14 ps in the calculation.[13] M_{mn} is given by

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

where e is the electronic charge, ψ_i $(i = m, n)$ is the wave function of the ith subband. They are obtained by solving the Schrödinger and Poisson equations self-consistently as [14]

$$-\frac{\hbar^2}{2}\frac{\mathrm{d}}{\mathrm{d}z}\left[\frac{1}{m^*(z)}\frac{\mathrm{d}}{\mathrm{d}z}\psi_i(z)\right] + [V(z) + \Delta E_c + V_{xc}(z) - e\phi_H(z)]\psi_i(z) = E_i\psi_i(z), \tag{3}$$

$$\frac{\mathrm{d}}{\mathrm{d}z}\left[\varepsilon_0\varepsilon_r\frac{\mathrm{d}}{\mathrm{d}z}\phi_H(z)\right] = -e\left[N_D^+(z) - n_{2D}(z)\right], \tag{4}$$

$$\begin{aligned} &V_{xc}(z) \\ &= -0.985\frac{e^2}{4\pi\varepsilon_0\varepsilon_r}n_{2D}^{1/3}(z) \\ &\times\left\{1 + \frac{0.034}{\alpha_H^* n_{2D}^{1/3}(z)}\ln\left[1 + 18.376a_H^* n_{2D}^{1/3}(z)\right]\right\}, \end{aligned} \tag{5}$$

where z is the space coordinate along the growth direction, $m^*(z)$ is the position-dependent effective mass, $V(z)$ is the applied voltage, ΔE_c is the conduction band offset, $\phi_H(z)$ is the Hartree potential due to the electrostatic interaction, $V_{xc}(z)$ is the exchange correlation potential,[15] $a_H^* = 4\pi\varepsilon_0\varepsilon_r\hbar^2/m^*(z)e^2$,[16] $N_D^+(z)$ is the ionized donor density and $n_{2D}(z)$ is the two-dimensional (2D) electron density in all subbands. Under the equilibrium condition, $n_{2D}(z)$ and N_i are given by the formulas as follows:[16]

$$\begin{aligned} &n_{2D}(z) \\ &= \sum_i n_{2D_i}(z) \\ &= \sum_i \frac{m_i^* kT}{\pi\hbar^2}|\psi_i(z)|^2\ln\left[1 + \exp\left(\frac{E_f - E_i}{kT}\right)\right], \end{aligned} \tag{6}$$

$$N_i = \int n_{2D_i}(z)\mathrm{d}z, \tag{7}$$

where k is the Boltzmann constant, T is the absolute temperature, m_i^* is the effective mass of electrons residing in the ith subband level (for simplicity, the same effective mass is used in the well) and E_f is the Fermi level. 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.

Especially, we include the depolarization effect and exciton-like effect in the intersubband transition energy (ΔE_{ij}).[17] The shifted intersubband transition energy $(\Delta E'_{ij})$ can be given by[18]

$$\Delta E'_{ij} = \Delta E_{ij}\sqrt{1+\alpha-\beta}, \tag{8}$$

$$\alpha = \frac{8\pi e^2(N_i - N_j)}{\varepsilon_r\Delta E_{ij}} \times\int_{-L_t/2}^{L_t/2}\mathrm{d}z\left[\int_{-L_t/2}^{z}\mathrm{d}z'\psi_j(z')\psi_i(z')\right]^2, \tag{9}$$

$$\beta = \frac{2(N_i - N_j)}{\Delta E_{ij}}\int_{-L_t/2}^{L_t/2}\mathrm{d}z\psi_j^2(z)\psi_i^2(z)\frac{\partial V_{xc}(n(z))}{\partial n(z)}, \tag{10}$$

where the quantities α and β are called the depolarization and the exciton shift, respectively; ψ_i is the wave function of the ith subband.

3. Results and discussion

In the calculation, the band gap is chosen to be 4.4 eV for $Al_{0.82}In_{0.18}N$[19] and 3.4 eV for GaN.[16] The minimum of the conduction band profile of $Al_{0.82}In_{0.18}N$/GaN SQW 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 $Al_{0.82}In_{0.18}N$/GaN SQW is zero. The structure of $Al_{0.82}In_{0.18}N$/GaN SQW used in the calculation is 6 nm $Al_{0.82}In_{0.18}N$ /L nm GaN, where L

is a variable. Figure 1 presents the schematic conduction band profile of the $Al_{0.82}In_{0.18}N$/GaN SQW and the moduli square of the wave function. The total polarization field discontinuities (ΔP) are assumed to be $\Delta P_1 = 0.037$ C/m^2, $\Delta P_2 = -0.037$ C/m^2. The doping concentration in the $Al_{0.82}In_{0.18}N$ barrier is assumed to be 5×10^{18} cm^{-3}. Dot A is the reference energy, which is defined as zero. There is no piezoelectric field in the $Al_{0.82}In_{0.18}N$/GaN system because of the lattice match of $Al_{0.82}In_{0.18}N$ and GaN. However, a large spontaneous polarization field exists in the $Al_{0.82}In_{0.18}N$/GaN system. As is shown in Fig. 1, the polarization-field-induced potential drops lead to the asymmetry of the conduction band profile.

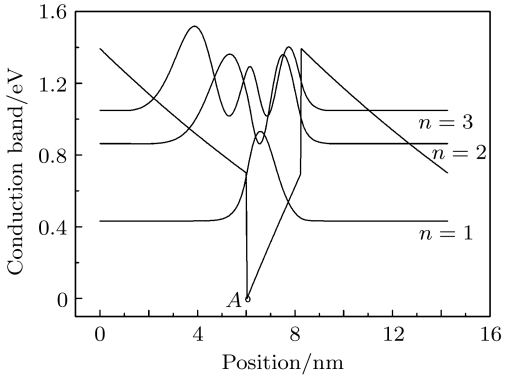


Fig. 1. Schematic conduction band profile of the $Al_{0.82}In_{0.18}N$/GaN SQW and the moduli square of the wave functions.

Figure 2(a) shows the wavelength of the 1–2 ISBT as a function of the thickness of the SQW L. As shown in Fig. 2(a), the wavelength of the 1–2 ISBT increases with L, due to the fact that with increasing L, the energy distance between subbands 1 and 2 decreases. The wavelength ranges from 2.88 μm to 3.59 μm, which is useful for mid-infrared communication systems. Figure 2(b) shows the moduli square of the dipole matrix of 1–2 ISBT as a function of the thickness of the SQW. It is clear that with the increase of the thickness of SQW, the moduli square of the dipole matrix of 1–2 ISBT increases with L at first and then reaches a relatively steady value. Figure 2(c) shows the total electrons residing in the subband 1 level as a function of the thickness of SQW. By increasing L, the total electrons residing in the subband 1 level decreases quickly. Figure 2(d) presents the absorption coefficients of 1–2 ISBT as a function of the thickness of the SQW. When L is smaller than 2.6 nm, the absorption coefficients of 1–2 ISBT increase and reach the climax when L is equal to 2.6 nm. However, when L is larger than 2.6 nm, the absorption coefficients of 1–2 ISBT decrease with L. This phenomenon can be explained as follows: from formula (1), we know that the absorption coefficients of the ISBT are mainly determined by three factors, the energy distance between the initial subband and the final subband,

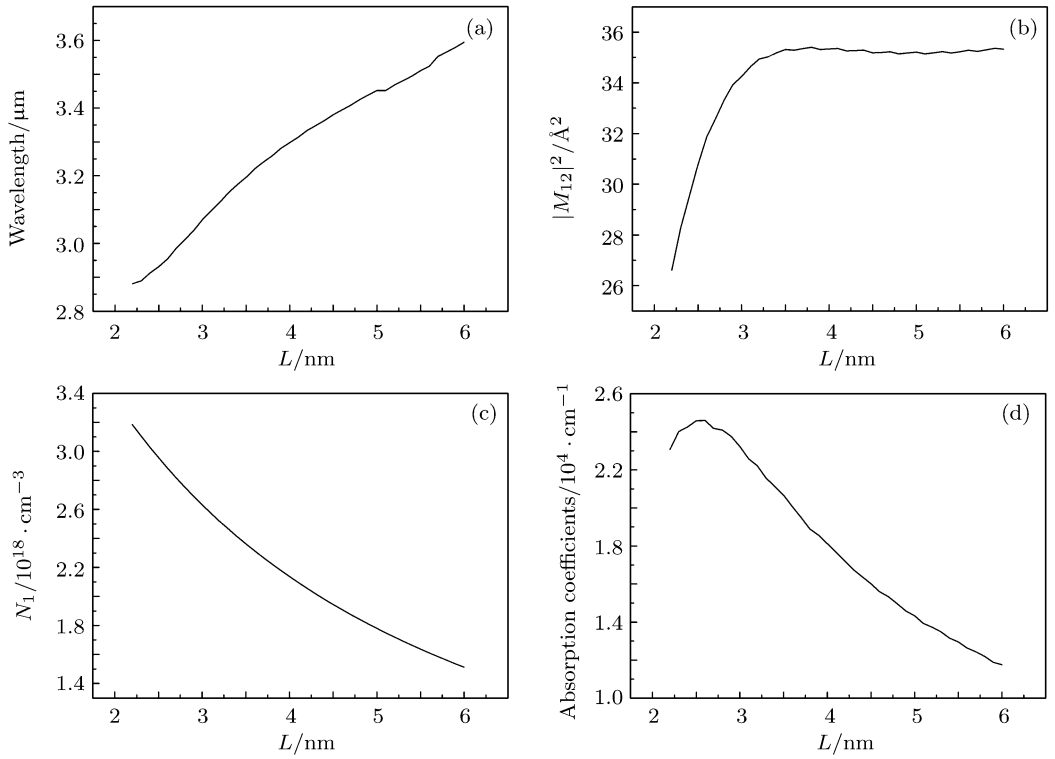


Fig. 2. (a) The wavelength of the ISBT between subbands 1 and 2, (b) the moduli square of dipole matrix of 1–2 ISBT, (c) the total electrons residing in the subband 1 level, and (d) the absorption coefficients of 1–2 ISBT as functions of the thickness of SQW.

the moduli square of dipole matrix and the total electrons residing in the initial and final subband. These three factors together influence the absorption coefficients of the ISBT. When L is smaller than 2.6 nm, the energy distance between subbands 1 and 2 decreases with L, while the moduli square of dipole matrix increases with L and the total electrons residing in subband 1 decrease with L. Moreover, the electron density in subband 2 is so insignificant that it is negligible. Therefore, the difference between N_1 and N_2 is mainly determined by N_1. It is believed that the increase of the moduli square of the dipole matrix and the decrease of the energy distance outdo the decrease of total electrons residing in subband 1 when L is smaller than 2.6 nm, which results in the fact that the absorption coefficients increase with L. However, with increasing L, the total electrons residing in subband 1 decrease so quickly that it becomes the dominant factor, which results in the absorption coefficients in subbands 1–2 decreasing with increasing L. It indicates that the thickness of SQW is an important factor in the design of $Al_{0.82}In_{0.18}N$/GaN SQW optoelectronic devices because it can impact the total electrons residing in subband 1, which has a significant influence on the absorption coefficients of ISBT.

Figure 3(a) plots the wavelength of the ISBT between subbands 1 and 3 as a function of the thickness of the SQW. As is shown in Fig. 3(a), the wavelength of the ISBT between subbands 1 and 3 decreases with L when L is smaller than 4 nm, while it increases with L when L is larger than 4 nm. The wavelength ranges from approximately 2.03 μm to nearly 2.11 μm, with a minimum when the thickness of the SQW is equal to 4 nm. This phenomenon can be explained as follows: with increasing L, the energy levels of both subband 1 and subband 3 decrease. However, the energy level of subband 3 decreases more slowly than that of subband 1 before L exceeds 4 nm. Therefore, the energy distance between subbands 1 and 3 will increase with L, which means that the wavelength of ISBT between subbands 1 and 3 decreases with L. The energy level of subband 3 decreases more quickly than that of subband 1 when L is larger than 4 nm, thus the energy distance between subbands 1 and 3 decreases with L, and the wavelength of ISBT between subbands 1 and 3 increases with L. Figure 3(b) shows the moduli square of the dipole matrix of 1–3 ISBT as a function of the thickness of the SQW. It is clear that with the increase of the thickness of SQW, the moduli square of dipole matrix of 1–3 ISBT decreases with L. Figure 3(c) shows the absorption coefficients of 1–3 ISBT as a function of the thickness of SQW. It is found that the absorption coefficients of 1–3 ISBT decrease with L. This can be explained as follows: the total electrons residing in subband 1 decrease with L (see Fig. 2(c)). The moduli square of the dipole matrix of 1–3 ISBT decreases with L. Though the energy distance between subbands 1 and 3 increases with L when L is larger than 4 nm, it is not the dominant factor determining the absorption coefficients. From formula (1), it is clear that the absorption coefficients of 1–3 ISBT will decrease with L.

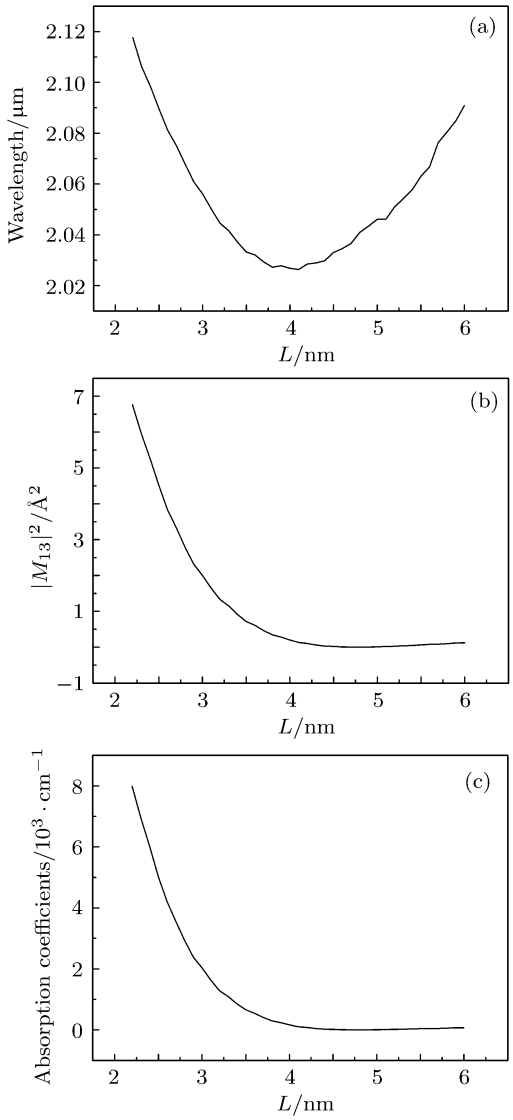


Fig. 3. (a) The wavelength of the ISBT between subbands 1 and 3, (b) the moduli square of the dipole matrix of 1-3 ISBT, and (c) the absorption coefficients of 1–3 ISBT as functions of the thickness of the SQW.

Figure 4 shows the absorption coefficients of the ISBTs of 1–2 and 1–3 as functions of the wavelength of the ISBTs, when L is 2.2 nm, which gives a pro-

file of the absorption coefficients of different wavelengths. The solid line represents the absorption coefficients as functions of the wavelength of the ISBTs with the exchange correlation potential V_{xc} taken into account, which is already considered in the above calculation. The dotted line represents the absorption coefficients as functions of the wavelength of the ISBTs without the exchange correlation potential V_{xc} taken into account. It is clear that there is a blue shift in the absorption spectrum with V_{xc} taken into account. We can conclude that the exchange correlation potential must be taken into account in the calculation. This can be explained as follows: A one-electron Schrödinger equation is used in the calculation. However, the real semiconductor is a many-electron system, in which the Pauli exclusion principle should be considered. Moreover, the electron density in the semiconductor is much smaller than that in the metal, resulting in that the shielding effect cannot shield the Coulomb interaction of the electrons and so the electrons will correlate with each other. Therefore, the Coulomb interaction of electrons must be considered. The interaction caused by the Pauli exclusion principle will result in exchange potential, and the influence of some electrons on the charge distribution in the whole system will result in correlation potential.[20] For the compensation of the one-electron approximation, we add the exchange correlation potential V_{xc} to the potential term of the Schrödinger equation.

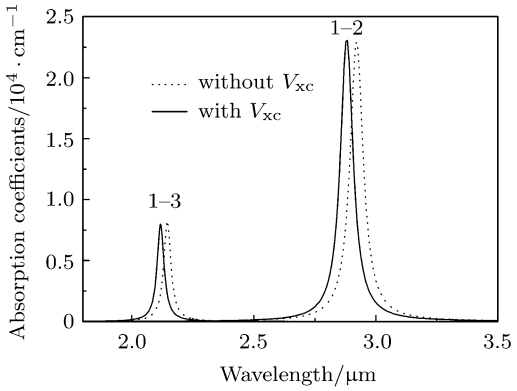


Fig. 4. The absorption coefficient of the ISBT of 1–2 and 1–3 as a function of the wavelength of the ISBT, when L is 2.2 nm.

4. Conclusions

In conclusion, the influence of width of a lattice-matched $Al_{0.82}In_{0.18}N$/GaN SQW on the absorption coefficients and wavelength of the ISBT has been investigated by solving the Schrödinger and Poisson equations self-consistently. The wavelength of 1–2 ISBT increases with L, ranging from 2.88 μm to 3.59 μm. The absorption coefficients of 1–2 ISBT increase with L at first and then decrease with L, with a maximum when L is equal to 2.6 nm. This is because the increase of the moduli square of the dipole matrix and the decrease of the energy distance are the dominant factors when L is smaller than 2.6 nm. However, the total amount of electrons residing in subband 1 decreases so quickly that it becomes the dominant factor after L exceeds 2.6 nm, which results in a decrease of the absorption coefficients of subbands 1 and 2 with L. The wavelength of 1–3 ISBT decreases with L at first and then increases with L, with a minimum when L is equal to 4 nm, ranging from approximately 2.03 μm to near 2.11 μm. The absorption coefficients of 1–3 ISBT decrease with L. The explanations for this phenomenon are as follows: even though the energy distance between subbands 1 and 3 increases with L when L is larger than 4 nm, it is not the dominant factor determining the absorption coefficients. Both the moduli square of the dipole matrix of 1–3 ISBT and the total amount of electrons residing in subband 1 decrease with L, which results in the fact that the absorption coefficients decrease with L. The results indicate that mid-infrared can be realized by the $Al_{0.82}In_{0.18}N$/GaN SQW. In addition, the wavelength and absorption coefficients of ISBT can be adjusted by changing the width of the SQW.

References

[1] Lei S Y, Shen B and Zhang G Y 2008 *Acta Phys. Sin.* **57** 2386 (in Chinese)
[2] He Z, Kang Y, Tang Y W, Li X and Fang J X 2006 *Chin. Phys.* **15** 1325
[3] Liu Z, Wang X L, Wang J X, Hu G X, Guo L C and Li J M 2007 *Chin. Phys.* **16** 1467
[4] Radovanovic J, Milanovic V, Indjin D and Ikonic Z 2002 *J. Appl. Phys.* **92** 7672
[5] Gmachl C, Frolov S V, Ng H M, Chu S N G and Cho A Y 2001 *Electron. Lett.* **37** 378
[6] Suzuki N and Iizuka N 1999 *Jpn. J. Appl. Phys.* Part 1 **36** 3222
[7] Gmachl C, Ng H M and Cho A Y 2000 *Appl. Phys. Lett.* **77** 334
[8] Suzuki N and Iizuka N 1997 *Jpn. J. Appl. Phys.* Part 2 **36** L1006
[9] Helman A, Tchernycheva M, Lusson A, Warde E, Julien F H, Moumanis Kh, Fishman G, Monroy E, Daudin B, Le D, Dang Si, Bellet-Amalric E and Jalabert D 2003 *Appl. Phys. Lett.* **83** 5196
[10] Kishino K, Kikuchi A, Knatawa H and Tachibana T 2002 *Appl. Phys. Lett.* **81** 1234

[11] Nicolay S, Carlin J F, Feltin E, Butté R, Mosca M, Grandjean N, Llegems M, Tchernycheva M, Nevou L and Julien F H 2005 *Appl. Physics. Lett.* **87** 111106
[12] Ahn D and Chuang S L 1987 *J. Quantum Electron.* **23** 2196
[13] Huang Y M and Lien C H 1995 *J. Appl. Phys.* **77** 3433
[14] Cen L B, Shen B, Qin Z X and Zhang G Y 2009 *Chin. Phys.* B **18** 3905
[15] Brey L, Dempsey J, Johnson N F and Halperin B I 1990 *Phys. Rev.* B **42** 1240
[16] Cen L B, Shen B, Qin Z X and Zhang G Y 2009 *J. Appl. Phys. Lett.* **105** 053106
[17] Manasreh M O, Szmulowicz F, Vaughan T, Evans K R, Stutz C E and Fischer D W 1991 *Phys. Rev.* B **13** 9996
[18] Ando T 1977 *Solid State Commun.* **21** 133
[19] Carlin J F, Zellweger C, Dorsaz J, Nicolay S, Chrismann G, Feltin E, Butté R and Grandjean N 2005 *Phys. Status Solidi* B **242** 2326
[20] Hedin L and Lundqvist B I 1971 *J. Phy.* C **4** 2064