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n doping effect modeling in 1.3 μm $GaN_{0.58y}As_{1-1.58y}Bi_y$/GaAs quantum wells

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HIGHLIGHTS

- Doping effect is modeled in 1.3 μm GaNAsBi/GaAs quantum wells (QWs).
- Owing to doping, a blue-shift of the fundamental transition energy was observed.
- Absorption peak intensity increases significantly with the rise of doping density.
- The well width dependence of the absorption coefficient is also studied.
- Bi composition was adjusted in order to obtain GaNAsBi/GaAs QWs operating at 1.3 μm.

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ABSTRACT

The effect of n doping on the band structure of lattice-matched GaNAsBi/GaAs quantum wells was investigated using a self-consistent calculation combined with the 16-band anti-crossing model. Bi/N incorporation and doping effects can offer a huge potential to engineer the electronic band structure of such materials suitable for the design of photodetectors and emitters operating at 1.3 μm. The increase of the doping density induces a blue-shift of the fundamental transition energy in the doping range between 6×10^{17} and 5×10^{18} cm^{-3}. The absorption spectra dependence on the well width are discussed. To maintain the fundamental transition fixed at the wavelength 1.3 μm, we have adjusted the Bi composition for the well width range between 4.5 and 10 nm with respect of the confinement conditions.

1. Introduction

The investigation of the electronic and optical properties of the III–V bismide–nitride alloys has attracted a great deal of attention due to its potential applications in optoelectronic devices. These alloys have been the focus of intensive research work in recent years owing to their interesting physical properties such as the temperature insensitive [1], the large band-gap reduction [2–6] and the strong spin–orbit splitting [7,8]. The effect of Bi incorporation into GaAs on the band-gap [9] and carrier effective mass [10] was theoretically studied using valence band anticrossing model. Wu et al. [11] have examined the band anticrossing (BAC) effect on the band-gap and electron effective mass of the highly mismatched $GaAs_{1-x}N_x$ alloys. Furthermore, the electronic band structure of GaNAsBi alloys was theoretically studied using BAC model at the wavelength region 1.3–1.55 μm [12,13]. Experimentally, Huang et al. [14] have grown $GaN_yAs_{1-x-y}Bi_x$ epilayer lattice-matched to GaAs substrate for the emission wavelength of 1.3 μm. They found that the photoluminescence peak energy for $GaN_yAs_{1-x-y}Bi_x$ is more temperature insensitive than the band gap of $In_{1-x}Ga_xAs_yP_{1-y}$. Moreover, quantum wells (QWs) based on dilute nitride such as GaInNAs/GaAs [15] and GaNAsSb/GaAs [16] are highly involved for the design of light-emitting diodes (LEDs) and photodetectors. Moreover, we have studied in a previous work [17] the electronic band structure of non-doped lattice-matched $GaN_xAs_{1-x-y}Bi_y$/GaAs QWs operating at 1.3 and 1.55 μm using BAC model. Besides, we have also investigated the effect of n-doped region on the electronic and optical properties of GaNAsBi/GaAs QWs [18]. On the other hand, various investigations reported the doping effect on radiatives transitions, oscillator strength and absorption coefficient for standard QWs such as AlAs/GaAs and AlGaAs/GaAs [19–21]. However, there are few studies which reported the doping effect on the optoelectronic properties of 1.3 μm

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$GaN_xAs_{1-x-y}Bi_y$/GaAs QWs.

The purpose of this work is to investigate the doping effect on the electronic band structure of $GaN_xAs_{1-x-y}Bi_y$/GaAs single quantum wells (SQWs). Particularly, we have studied the doping density dependence of the subbands, the confined electron density and the absorption coefficient. Further, we have examined the well width dependence on the absorption coefficient magnitude at the allowed transitions for $GaN_xAs_{1-x-y}Bi_y$/GaAs SQWs operating at 1.3 μm. Finally, the Bi composition is adjusted for different well width values in order to keep the fundamental transition fixed at the wavelength 1.3 μm.

2. Theoretical approach

In our previous work, we have performed a self-consistent calculation combined with (16×16) BAC model to examine the electronic band structure of n–i doped $GaN_xAs_{1-x-y}Bi_y$/GaAs QWs operating at 1.55 μm [18]. Moreover, lattice-matched $GaN_{0.58}As_{1-1.58y}Bi_y$/GaAs QWs can reach the wavelength 1.3 μm using the well width L_w and Bi composition y as 4.5 nm and 0.05 (*i.e.* N composition $x=0.03$) respectively [17]. Band structure of GaNAsBi/GaAs QWs can be described by the total Hamiltonian $H = H_{\|} + H_z$ [17, 22], where $H_{\|} = -\frac{\hbar^2}{2m^*_{\|i}}\nabla^2_{\|}$ is the Hamiltonian of system in a direction parallel to the GaNAsBi–GaAs interface. $m^*_{\|i}$ ($i = e$ for electron and h for heavy hole) is the carrier effective mass in $\boldsymbol{k}_{\|}$-direction. $H_z = -\frac{\hbar^2}{2}\nabla_z\frac{1}{m^*_{ij}(z)}\nabla_z + V(z)$ is the Hamiltonian of system in quantizing z-direction where $V(z)$ is the total potential energy. The coupled Schrödinger–Poisson equations are written as:

$$\left(-\frac{\hbar^2}{2}\nabla_z\frac{1}{m^*_{ij}(z)}\nabla_z + U_B(z) + U_H(z) + U_{xc}(z)\right)\varphi_j(z) = E_j\,\varphi_j(z) \quad (1)$$

$$\frac{d^2U_H(z)}{dz^2} = \frac{e^2}{\varepsilon_0\varepsilon_r}(N_d(z) - n(z)) \quad (2)$$

E_j and $\varphi_j(z)$ are the eigenvalues and eigenvectors of H_z respectively. The envelope wavefunctions $\varphi_j(z)$ satisfy the boundary condition at the interfaces ($z = 0$) and ($z = L_w$). In the case of non-doped GaNAsBi based-QWs, $V(z)$ is restricted to the band discontinuity $U_B(z)$ between the GaAs barrier and GaNAsBi well. For n–i doped GaNAsBi/GaAs QWs, the total potential energy is the sum of the band discontinuity $U_B(z)$, the Hartree potential $U_H(z)$ and the exchange-correlation potential $U_{xc}(z)$. $U_H(z)$ is obtained by solving the Poisson equation discretized using the finite differences method (FDM) taking into account the boundary conditions. The exchange-correlation potential $U_{xc}(z)$ is induced by the many-body effects [18,23]. $N_d(z)$ and $n(z)$ are the donor and confined electron density respectively. e is the absolute value of the electron charge and $\varepsilon_0\varepsilon_r$ is the local dielectric constant of the medium. The Eqs. ((1) and 2) were discretized along the confinement z-direction using the FDM.

The iterative process is used to solve the coupled Schrödinger–Poisson equations simultaneously until the convergence is completed. The computed relative variation of the electron density at the convergence is less than 10^{-9}. More calculation details of the iterative procedure as well as the inter-band absorption coefficient, the oscillator strength and the carrier effective mass are reported in the references [17,18,24].

3. Results and discussion

The study of the band-gap energy and carrier effective mass of $GaN_xAs_{1-x-y}Bi_y$ bulk in our previous work [12] stands as a starting point for the band structure calculation of such quantum structures. Then, we have theoretically investigated the electronic band structure of non-doped $GaN_xAs_{1-x-y}Bi_y$/GaAs QWs using (16×16) BAC model [17]. To obtain only one allowed radiative transition T_{e1-h1} fixed at 1.3 μm (*i.e.* 0.95 eV), between the electron subband $e1$ and the heavy hole subband $h1$, the used well width L_w and Bi composition y are equal to 4.5 nm and 0.05 (*i.e.* $x=0.03$) respectively. The computed carrier effective masses relative to the conduction and valence bands edges of $GaN_{0.03}As_{0.92}Bi_{0.05}$ bulk are 0.057 m_0 and 0.492 m_0 respectively, m_0 being the free electron mass. The calculated conduction and valence bands discontinuities ΔE_c and ΔE_v are equal to 0.43 and 0.23 eV respectively. The computed absorption coefficient at the wavelength 1.3 μm is found to be 4.4×10^4 cm^{-1} [17]. Bismuth introduces two localized levels E_{Bi} and E_{Bi-so} located respectively at 0.40 and 1.90 eV below the GaAs valence band edge [2]. Nitrogen localized level E_N is positioned at 0.23 eV above the GaAs conduction band edge [11]. The subbands energies related to electron and holes are denoted as ei and hj respectively. The oscillator strength of the transition energy T_{ei-hj} is given by the following expression [25]: $f_{ei-hj} = E_P/T_{ei-hj}\left|\Gamma_{ei-hj}\right|^2$ where $E_P = \frac{2}{m_0}\left|\langle u_c|p_z|u_v\rangle\right|^2$ is the Kane parameter calculated within the ***k.p*** theory [24] and $\left|\Gamma_{ei-hj}\right| = \left|\langle\varphi_{ei}|\varphi_{hj}\rangle\right|$ is the modulus of the wavefunctions overlapping.

In order to enhance the absorption near the wavelength 1.3 μm, we have studied the n doping effect on the electronic and optical properties of $GaN_xAs_{1-x-y}Bi_y$/GaAs QWs. In Fig. 1a, we have plotted the energy band diagrams in z-confinement direction of non-doped (i–i–i) and n doped well (i–n–i) $GaN_{0.03}As_{0.92}Bi_{0.05}$/GaAs SQWs. The used donor density N_d is equal to 5×10^{18} cm^{-3}. For (i–i–i) SQWs, the computed fundamental transition T_{e1-h1} is equal to 0.95 eV (*i.e.* 1.3 μm). The calculated electron subband $e1$ is situated at 1.15 eV and two heavy holes subbands $h1$ and $h2$ are positioned at 0.19 and 0.09 eV respectively. The carrier effective masses m^*_{e1}, m^*_{h1} and m^*_{h2} at the zone center are 0.108 m_0, −0.217 m_0 and −0.103 m_0 respectively. The calculated oscillator strength is equal to 13.92. On the other hand, the energy band diagram of n doped well (i–n–i) SQWs shows that the T_{e1-h1} shifts slightly 10 meV to higher energies compared to the fundamental transition 1.3 μm (*i.e.* 0.95 eV) in the case of the non-doped (i–i–i) SQWs. This shift is due to the doping effect on the band-bending at the GaNAsBi–GaAs interface. In other study, Kim and Park [26] have investigated the effect of modulation doping on the optical properties of $GaAs_{0.76}Sb_{0.24}/In_{0.26}Ga_{0.74}N_{0.06}As_{0.94}$/GaAs QWs. They found that the fundamental transition shifts 20 meV to higher energies with the increase of the in-plan carrier density from 10^{12} to 5 10^{12} cm^{-2}. In addition, a transition energy shift 30 meV is stated in the study of the multi-color CdS/ZnSe quantum structures when the donor density rises from 5×10^{17} to 3.5×10^{18} cm^{-3} [27]. Note that the dissimilarity of the transition wavelength shift value in the case of $GaN_{0.03}As_{0.92}Bi_{0.05}$/GaAs QWs compared to other systems may be due to the difference in their physical properties for example the doping density, confining potential and carrier effective masses. Furthermore, for (i–n–i) SQWs the computed electron subband $e1$ is located at 1.14 eV. The two heavy holes subbands $h1$ and $h2$ are situated at 0.18 and 0.08 eV respectively. The obtained Fermi level E_F and the oscillator strength are found to be 1.26 eV and 13.91 respectively. The calculated carrier effective masses m^*_{e1}, m^*_{h1} and m^*_{h2} at the zone center are 0.107 m_0, −0.118 m_0 and −0.086 m_0 respectively. Fig. 1b shows the band structure and confined electron and heavy holes subbands ($e1$, $h1$ and $h2$) in $\boldsymbol{k}_{\|}$-direction of non-doped (i–i–i) and n doped well (i–n–i) of $GaN_{0.03}As_{0.92}Bi_{0.05}$/GaAs SQWs. The nitrogen E_N and bismuth E_{Bi} localized levels at −0.40 and 1.65 eV are