Physica E 43 (2011) 919–923

Contents lists available at ScienceDirect

Physica E

journal homepage: www.elsevier.com/locate/physe

The comparison of the band alignment of GaInAsN quantum wells on GaAs and InP substrates for (0 0 1) and (1 1 1) orientations

K. Köksal [a,*], B. Gönül [b]

[a] Physics Department, BitlisEren University, 13000 Bitlis, Turkey
[b] Department of Engineering Physics, University of Gaziantep, 27310 Gaziantep, Turkey

ARTICLE INFO

Article history:
Received 28 April 2010
Received in revised form
1 November 2010
Accepted 7 November 2010
Available online 18 November 2010

ABSTRACT

The aim of this paper is to examine the effect of growth orientation and dilute nitride on the band alignment of GaInAs quantum wells on GaAs and InP substrates by means of model solid theory. The study provides a comparison of the band alignment and the strained band gap of the related GaInAsN QWs in (1 1 1) and (0 0 1) orientation. Our calculated results show that although 111-oriented GaInAsN QWs enables to reach the longer wavelengths, the conduction band offset gets shallow than that of the 001-oriented ones.

1. Introduction

Recently, there has been much interest in dilute nitride compound semiconductors of GaInAsN since the incorporation of nitrogen in GaInAs has a profound influence on the electronic properties of these materials and allows widely extended band structure engineering. Numerous experimental and theoretical works have been published about that GaInAsN on GaAs substrates [1–4]. The larger conduction band offset which results in improved electron confinement and decreased electron spill out at/above room temperature is one of the most important advantages of this material as compared to the most commonly used GaInAsP/InP systems. In our previous work [5], we presented band alignment properties of GaInAsN on GaAs substrates for (0 0 1) orientation.

GaInAsN alloy also can be grown without any strain on common substrate InP for (0 0 1) orientation. The addition of nitrogen to lattice-matched or compressively strained GaInAs on InP results in a sizeable reduction of the band gap energy of the resulting InP-based GaInAsN layer, accompanied by a reduction in the lattice constant as it is similar to dilute GaInAsN on GaAs. Strained and lattice-matched $Ga_{1-x}In_xAs_{1-y}N_y$ alloys on InP can also extend the wavelength of photonic device operation beyond that accessible to the $Ga_{1-x}In_xAs_{1-y}N_y$/InP system. Increasing In content in $Ga_{1-x}In_xAs$ on InP beyond 53% results in a decrease of the band gap energy which, however, is partially offset by increasing compressive strain. Incorporating N to $Ga_{1-x}In_x$ As reduces the band gap energy even further. Moreover, the incorporation of N compensates for compressive strain in the case of $x \succ 0.53$ and introduces tensile strain in the case of $x \preceq 0.53$, resulting an additional reduction of band gap energy for both cases. There are limited works so far on the growth of strained GaInAsN on InP substrates [6–12]. We have investigated band alignment properties of strained and strain-compensated GaInAsN QWs on InP substrate for (0 0 1) orientation in our previous works [5,13].

GaInAsN alloy can be grown on 1 1 1-oriented substrates. It is known that the molecular beam epitaxy growth of strained zincblende materials on {1 1 1} orientation shows some interesting properties. In particular, strained QWs grown in these orientations are piezoelectric and pyroelectric [14,15] such that their optical transitions are red-shifted relatively to the (0 0 1) ones. The {1 1 1} strained layers also show larger critical thicknesses for strain relaxation compared to (0 0 1) oriented ones [16,17]. These two properties combine and allow the achievement of strained QWs emitting at longer wavelength than that for 001-oriented ones. Blanc et al. [18] has shown that the growth orientation has a great influence on the structural and optical characteristics of N diluted alloys, and the use of alternative growth orientations could help to get a better insight into the peculiar properties of these materials, which open a new challenge to GaAs optoelectronics.

In this paper we aim to investigate the effect of growth orientations, substrates, nitrogen and indium concentrations on the band gap and band offsets of GaInAsN. Band alignment calculations of the GaInAsN/GaAs and GaInAsN/InP for (0 0 1) and (1 1 1) orientations are performed by means of using model solid theory. For laser systems, the material parameters except for the band gap energies are linearly interpolated from those of binary materials [19]. The calculation of bulk band gap energy of GaInAsN is performed by means of using band anti crossing model.

* Corresponding author at: Physics Department, BitlisEren University, 13000 Bitlis, Turkey.
E-mail address: kkoksal@bitliseren.edu.tr (K. Köksal).

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doi:10.1016/j.physe.2010.11.004

2. Theoretical models

2.1. Band anti-crossing model

It has been reported that band anticrossing (BAC) model [20] can describe the composition dependence of band gap energy of GaInAsN on GaAs substrates. The proposed model has particular importance since, despite its simplicity, it manages to explain the basic properties of the material and to provide analytical expressions, such as conduction band edge dispersion relations and electron effective mass. The BAC has been successfully used to describe the dependences of the upper and lower subband energies on nitrogen concentration. The model is based on the interaction of the lowest conduction band with the highly localized N-induced energy level E_N, located 1.64 eV above the valence band edge of GaAs.

It has been shown that an anti-crossing interaction of the localized N states with the extended state of GaAs or GaInAs leads to a characteristic splitting of the conduction band into two non-parabolic subbands [21]. The low energy edges of the subbands are given by

$$E_{\pm} = (E_N + E_M \pm [(E_N - E_M)^2 + 4V_{MN}^2]^{1/2})/2 \quad (1)$$

where E_M and E_N are the energies of the extended state and of the N level relative to the top of the valence band (VB), respectively. $V_{MN}(=C_{MN}\sqrt{y}\text{eV})$ [22], where y is the N composition, is the matrix element of the term describing the interaction between localized N states and the extended states. The predicted splitting of the conduction band into subbands has been confirmed experimentally [20]. The nitrogen level dependence on the nitrogen composition is $E_N = 1.52 - 3.9y$ [23] The conduction band energy E_M of the matrix semiconductor is taken to vary in the presence of nitrogen as $E_M = E_0 - 1.55$ where E_0 is the energy in the absence of nitrogen [23]. We have used the band anticrossing model with an interaction parameter of $C_{MN} = 2.3$ eV [10] for strained GaInNAs quantum wells on InP substrates and $C_{MN} = 2.7$ eV for compressively strained GaInNAs quantum wells on GaAs substrates. The interaction parameter is an average value for high indium containing samples taken from Serries et al. [9].

For the band structures of laser systems, the material parameters except for the band gap energies are linearly interpolated from those of the binary materials [19] and these are tabulated in 1. The bulk band energy of $Ga_{1-x}In_xN_yAs_{1-y}$ is calculated by means of Eq. (1).

2.2. Model solid theory for (0 0 1) and (1 1 1) orientations

The relative band alignment of the band edges between quantum well and barrier is the total band discontinuity distributed over the conduction and valence bands, ΔE_c and ΔE_v, respectively. The band discontinuity depends on the semiconductors and the amount of mismatch strain at the interface. It has been commonly accepted that the nitrogen incorporation mainly affects the conduction band states of the GaInNAs alloys leading to an increase in the conduction band offset Q_c, and a small discontinuity in the valence band edge [24]. According to Van de Walle's model solid theory [25] the band offset ratio for conduction and valence band, $Q_{c,v}$, is determined by discontinuity fractions of $\Delta E_{c,v}/\Delta E_g$. The energy of the potential barrier, ΔE_g is determined from the difference between the bulk bandgap energy of the barrier layers and the strained bandgap energy of the active layer. The effect of strain is calculated as

$$\varepsilon_{\parallel} = \varepsilon_{xx} = \varepsilon_{yy} = \frac{a_s - a_e}{a_e} \quad (2)$$

$$\varepsilon_{zz} = -\frac{2C_{11} + 4C_{12} - 4C_{44}}{C_{11} + 2C_{12} + 4C_{44}}\varepsilon_{\parallel} \quad (3)$$

where a_s is the lattice constant of substrate and a_e is the lattice constant of quaternary epitaxial layer. The conduction band position can be calculated by simply adding the strained bandgap energy to the valence band position. The unstrained valence band-edge of the active region material is set as the reference energy of zero. The valence band position is given by

$$E_v(x,y) = \begin{cases} E_{v,av}(x,y) + \dfrac{\Delta_0(x,y)}{3} + \delta E_{hh}(x,y) & \text{for } hh \\ E_{v,av}(x,y) + \dfrac{\Delta_0(x,y)}{3} + \delta E_{lh}(x,y) & \text{for } lh \end{cases} \quad (4)$$

where $E_{v,av}(x,y)$ is the average valence subband energy and Δ_0 is the spin–orbit split-off band energy. These values are obtained by linear interpolation method where the binary values are listed in Table 1. The conduction band is shifted by the energy $\delta E_c(x,y)$

$$\delta E_c(x,y) = 2a_c\left(1 - \frac{C_{12}}{C_{11}}\right)\varepsilon_{\parallel} \quad \text{for (0 0 1)} \quad (5)$$

$$\delta E_c(x,y) = a_c(2\varepsilon_{xx} + \varepsilon_{zz}) \quad \text{for (1 1 1)} \quad (6)$$

the valence bands are shifted by energy, $\delta E_{hh}(x,y)$ and $\delta E_{lh}(x,y)$

$$\begin{aligned} \delta E_{hh}(x,y) &= -P_s - Q_s \\ \delta E_{lh}(x,y) &= -P_s + Q_s \end{aligned} \quad (7)$$

where

$$\begin{aligned} P_s &= -2a_v\left(1 - \tfrac{C_{12}}{C_{11}}\right)\varepsilon_{\parallel} \\ Q_s &= -b\left(1 + \tfrac{2C_{12}}{C_{11}}\right)\varepsilon_{\parallel} \end{aligned} \quad \text{for (0 0 1)} \quad (8)$$

$$\begin{aligned} P_s &= -a_v(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) \\ Q_s &= -\tfrac{d}{2\sqrt{3}}(\varepsilon_{xx} + \varepsilon_{yy} - 2\varepsilon_{zz}) \end{aligned} \quad \text{for (1 1 1)} \quad (9)$$

where a_c and a_v are the conduction- and valence-band hydrostatic deformation potentials, b is the valence band shear deformation potential and C_{11} and C_{12} are elastic stiffness constants. The strained band gaps can then be expressed as

$$\begin{aligned} E_{c-hh}(x,y) &= E_g(x,y) + \delta E_c(x,y) - \delta E_{hh}(x,y) \\ E_{c-lh}(x,y) &= E_g(x,y) + \delta E_c(x,y) - \delta E_{lh}(x,y) \end{aligned} \quad (10)$$

The conduction band position is

$$E_c(x,y) = \begin{cases} E_v(x,y) + E_{c-hh}(x,y) & \text{for } hh \\ E_v(x,y) + \delta E_{c-lh}(x,y) & \text{for } lh \end{cases} \quad (11)$$

The conduction band offset is given by

$$\frac{\Delta E_c}{\Delta E_g} = 1 - \frac{E_v^w - E_v^b}{E_g^b - E_g^w} \quad (12)$$

Table 1
Some material parameters which have been used in calculations of band alignment.

Material	GaAs	GaN	InAs	InP	InN
a_e (Å)	5.6533	4.5	6.0584	5.8697	4.98
E_g (eV)	1.424	3.299	0.417	1.4236	0.78
Δ_0(eV)	0.34	0.017	0.39	0.108	0.005
a_c (eV)	−7.17	−6.71	−5.08	–	−2.65
a_v (eV)	−1.16	−0.69	−1.0	–	−0.7
C_{11}(Gpa)	1221.0	293.0	832.9	–	187.0
C_{12} (Gpa)	566.0	159.0	452.6	–	125.0
C_{44} (Gpa)	600.0	432.2	395.0	–	86.0
b (eV)	−2.0	−2.0	−1.8	–	−1.2
d (eV)	−4.8	−3.7	−3.6	–	−9.3
$E_{v,av}$(eV)	−6.92	–	−6.67	−7.04	–