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Atomistic calculations of Ga(NAsP)/GaP(N) quantum wells on silicon substrate: Band structure and optical gain

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Band structure calculations of strained Ga(NAsP) quantum wells are performed within the framework of the extended-basis $sp^3d^5s^*$ tight-binding model. The nitrogen contribution is taken into account by introducing an additional s_N orbital into the tight-binding basis. Biaxial strain effects on the band alignment of bulk Ga(NAsP) is studied for the ultra-diluted regime. We demonstrate a good agreement with experimental data both for transition energies and optical gain in Ga(NAsP) quantum wells. The effect of N incorporation in the laser active areas is simulated. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.3694028>]

The monolithic integration of III-V materials on silicon substrate has received a considerable interest¹ in recent years. Among the different strategies, the pseudomorphic approach should bypass high defect densities encountered in both GaAs and InP layers grown on a Si substrate.² This issue is prohibitive to develop both types of applications: efficient electrically pumped lasers on silicon and high efficiency multijunction solar cells. Recently, the epitaxial growth on Si substrate of the quasi lattice-matched GaP and perfectly lattice-matched GaP_{0.02} layers has been greatly improved³⁻⁵ allowing for GaPN-based active areas to efficiently emit light.⁶ Among them, quaternary Ga(NAsP) quantum wells (QWs) have shown to be reliable in both electrically pumped laser on GaP (Ref. 7, at room temperature) and Si (Ref. 8, below 150 K) substrates. Nevertheless, to optimize the design of an efficient laser structure, modelling of optical properties is of crucial importance. For the past decade, the diluted nitride alloys have been well studied through various theoretical strategies. Polymorphous models, such as empirical pseudopotentials method⁹ (EPM) or supercell tight-binding (TB) calculations,¹⁰ predicted the energetic position of nitrogen-related levels (localised and cluster states) for both ternaries GaAsN and GaPN. On the other hand, the band anticrossing (BAC) model,¹¹ based on the repulsion of a N-related level with the Γ -level of the host material, has been widely used because of its simplicity and its qualitative agreement with experimental observations (for instance, red shift of the bandgap and effective mass evolution with N content). All these models agree on the conclusion that the different behaviours between GaAsN and GaPN are explained by the difference of the host material band gap nature (direct for GaAs and indirect for GaP) and by the position of the N-related level relative to the conduction band (CB) (above the conduction band of GaAs and below that of GaP).¹² Because of their computational complexity, polymorphous models have not been employed for the quaternary Ga(NAsP) bulk alloy or quantum heterostructures. Meanwhile, the parameterization of the BAC description of Ga(NAsP) has been proposed from parameters of ternaries

GaAsN and GaPN (Ref. 13), and an 8-band $\mathbf{k}\cdot\mathbf{p}$ model has been modified to include the two additional BAC bands.¹⁴ Nevertheless, the current theoretical results on Ga(NAsP) QWs suffer from the lack of biaxial strained effects or lateral valleys consideration.^{14,15}

In this paper, we consider the extended-basis $sp^3d^5s^*$ tight-binding model which has proved to provide a band structure description with submillielectron volt precision throughout the Brillouin zone of binary semiconductors¹⁶ including quantum heterostructures and surface.^{17,18} We model our ternaries (GaAsP) by a linear interpolation of all TB parameters but allow for a parabolic contribution of the relevant two-center parameters determining the experimental band positions at the Γ , X, and L points. Strain effects are taken into account in the same way of smaller TB models by using a generalisation of Harrison's d^{-2} law for hopping integrals known to be reliable for strained III-V QW structures.¹⁹ The valence band offsets (VBOs) are taken from recent *ab initio* calculations.²⁰ In order to adapt the model to diluted nitride alloys, we follow the work of Shtinkov *et al.* where a s_N orbital has been added.²¹ This spherical state represents a nitrogen-related level which can interact with the nearest-neighbour atomic shell. The resulting $sp^3d^5s^*s_N$ Hamiltonian of the diluted nitride alloy is different from the $sp^3d^5s^*$ Hamiltonian of the host material by only two additional parameters which are similar to the BAC parameters: the energy of the s_N state, namely, E_s^N , and the coupling parameter $s_c s_N \sigma$.²¹ This model has been employed to study (In)GaAsN/GaAs heterostructures or GaPN alloy and can explain some experimental features such as E_1 , E_2 , or E^* transitions inaccessible to BAC-derived models which are limited to the center of the Brillouin zone.^{22,23} The additional parameters used in this work are

$$E_s^N = 1.65 \text{ eV and } s_c s_N \sigma = -1.04\sqrt{x} \text{ eV for GaAs}_{1-x}\text{N}_x,$$

$$E_s^N = 2.19 \text{ eV and } s_c s_N \sigma = -1.09\sqrt{x} \text{ eV for GaP}_{1-x}\text{N}_x.$$

E_s^N is set with regard to VBO to fix the position of the nitrogen level independent of the host material.²⁰ $s_c s_N \sigma$ is chosen to match results with E+ and E- transitions of bulk GaAsN and GaPN in the BAC model.¹⁴ The value of this coupling

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parameter depends very slightly of the host material because of the nature of the localised N-level in bulk semiconductors.

Fig. 1 shows the calculated VB and CB of GaAsP:N as a function of the As content for two configurations: unstrained (dashed lines) and strained on Si (001) (solid lines). The N concentration is set to be infinitesimally low, and the N-level is represented by the dash-dotted line. The energy reference is the VB maximum of bulk GaP. We found a direct-indirect band gap crossover in the unstrained GaAsP alloy occurring for about 50% of As content, in agreement with experiment.²⁴ The position of the N-level relative to the CB is located 170 meV under the X point of unstrained GaP and 131 meV above the Γ point of unstrained GaAs. The L-band is not represented for clarity. The CB minimum of unstrained GaAs_yP_{1-y} crosses the N-level for $y \approx 0.75$, and the maximum separation between the N-level and the CB edge of unstrained GaAs_yP_{1-y} is obtained for $y \approx 0.45$. This is consistent with the early results of Groves.²⁵ For GaAsP:N strained on Si (001), the VB maximum results from the heavy-hole states. The degeneracy of X CB is also lifted with an upper Xz level and lower Xxy valleys as a direct consequence of the compressive strain. The Γ CB is found above the Xxy CB for all composition range, in agreement with the results of Prieto *et al.*²⁶ for the case of GaAs strained layer on GaP(001) which is observed slightly indirect near the X-point. The N-level is insensitive to strain as in reported previous works^{27,28} and lies below the CB of strained GaAsP whatever the content.

Fig. 2 shows the effect of N concentrations on the Γ CB levels in a diluted regime. As predicted by the BAC model, the N level interacts with the Γ band of the host strained material to form two subbands Γ^- and Γ^+ . The other bands are not represented for clarity because their change in energy compared to their position in Fig. 1 is weak. We just briefly describe the major behaviours. The VB and the Xxy and Xz conduction valleys are just slightly affected by a weak decrease of the compressive strain due to the nitrogen incorporation. Finally, the L CB states undergo a similar but weaker behaviour than the Γ state with the appearance of two bands, namely, L+ and L-, which derive from the inter-

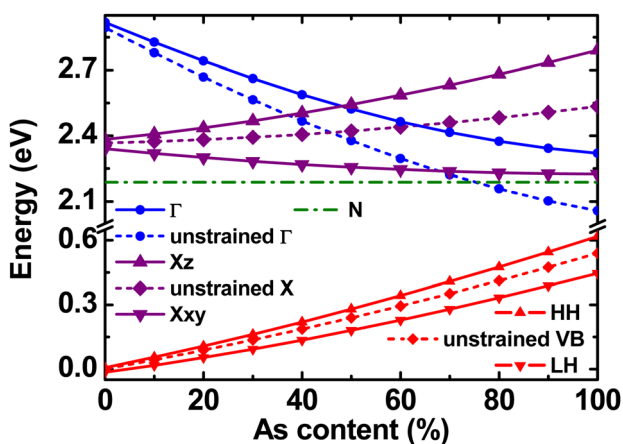


FIG. 1. (Color online) Conduction and valence bands of bulk GaAsP:N with a N concentration infinitesimally low at 0K. Dashed lines represent the unstrained case, solid lines represent the biaxially strained case, and the dash-dotted line represents the position of the N-level. The L band is not represented for clarity.

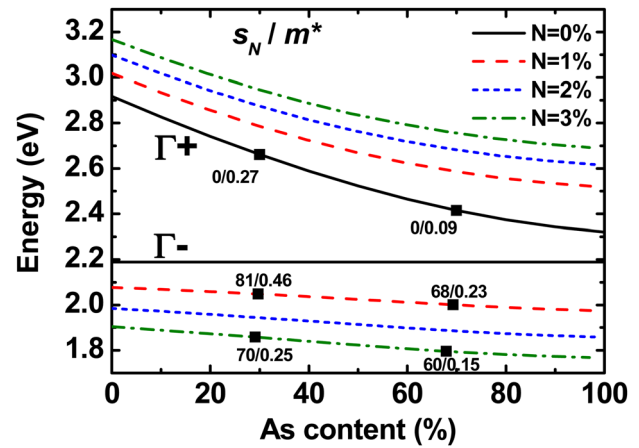


FIG. 2. (Color online) Γ^- and Γ^+ conduction bands for bulk Ga(NAsP) biaxially strained at different nitrogen concentrations at 0K. The energy reference is the same as in Fig. 1. The percentage of s_N contribution to the wave function is represented by the first number. The second number is the effective mass in the (100) direction in units of free electron mass m_0 .

action between the L bands of the host material and the N-related level. The relative contribution in percent of the s_N orbital to the electronic wave functions²¹ is also shown in Fig. 2 for different N and As contents. The Γ^- band evidences a predominant s_N character as a consequence of the lower energetic position of the N-level relative to the Γ band of strained GaAsP. This result is in contradiction with recent papers^{14,15} where the biaxial strain or lateral valleys are not taken into account. The second number is the effective mass in the (100) direction. The Γ^- band evidences a strong effective mass because of its N character but it decreases with N content because of the position of the N level below the Γ band of the host material.

Fig. 3 shows the calculated band structure of a 2.7 nm thick GaN_{0.005}As_{0.7}P_{0.295} QW with GaP_{0.995}N_{0.005} barrier strained on GaP (001) close to Brillouin zone center. Photoluminescence has been demonstrated for such a structure in our last work.²⁹ The envelope wave functions of the first conduction and valence subbands are represented in the two

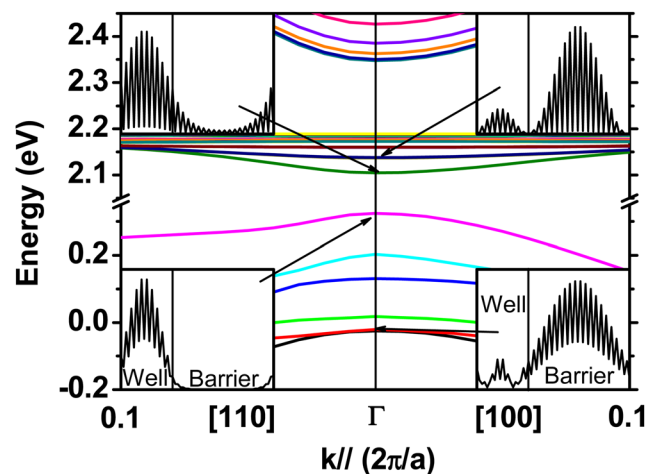


FIG. 3. (Color online) Band structure of a 2.7 nm thick (GaN_{0.005}As_{0.7}P_{0.295})/GaP_{0.995}N_{0.005} QW biaxially strained on GaP substrate at 0K. The envelopes wave functions of the conduction and valence band extrema for the well and the barrier are represented in insets. The energy reference is the same as in Fig. 1.

insets on the left. The envelope wave functions of the CB minimum and VB maximum of the barrier are plotted in the insets on the right evidencing a type-I in real space. The energy transitions in the well and in the barrier are equal to 1.78 eV and 2.16 eV. This is consistent with the photoluminescence spectrum at 12 K which exhibits a QW peak at 1.73 eV and a broad barrier peak located at 2.15 eV.²⁹

The optical gain is analysed for an experimental structure which exhibits a lasing effect.³⁰ The material gain is calculated for a 8 nm thick GaN_xAs_{0.92-x}P_{0.08} QW with GaP barriers on GaP substrate, according to the following expression:

$$g(E) = \frac{\pi \hbar e^2}{n_r c \epsilon_0 m_0^2 E} \times \frac{1}{L} \int \frac{d^2 k}{4\pi^2} |\hat{e} \cdot \mathbf{p}_{vc}(\mathbf{k})|^2 \left(f(E_c(\mathbf{k}), E_{fc}, T) - f(E_v(\mathbf{k}), E_{fv}, T) \right) \frac{1}{\sigma \sqrt{2\pi}} \exp\left(-\frac{(E - E_{vc}(\mathbf{k}))^2}{2\sigma^2} \right),$$

where L is the QW thickness, f the Fermi-Dirac distribution, E_{fc} and E_{fv} the quasi-Fermi levels, $\sigma = 5$ meV the standard deviation associated with a Gaussian lineshape broadening, and $E_{vc}(k) = E_c(k) - E_v(k)$ the different transitions between CB and VB. n_r is set equal to the GaAs_{0.92}P_{0.08} static refractive index. The dipole matrix elements $|\hat{e} \cdot \mathbf{p}_{vc}(\mathbf{k})|^2$ are calculated using a derivation of the TB Hamiltonian.³¹ Results for TE polarisation, room temperature, and various N concentrations are represented in Fig. 4 (the carrier density is $4 \times 10^{18} \text{ cm}^{-3}$). Increasing N content is found to increase the maximum of the gain. Experimentally, the energy position of the gain maximum was reported at 1.30 eV at 293 K and the N composition was assumed to be equal to 3.5%. Nevertheless, as quoted by the same authors,¹⁵ the experimental determination of Ga(NAsP) quaternary alloy composition is very difficult. According to our calculations, a maximum gain at 1.30 eV rather matches with a somewhat lower N content between 2% and 2.5%. Taking into account mirror losses and optical confinement factor, a lower limit for the material gain of about 240 cm^{-1} was proposed experimentally. The theoretical calculation leads to a maximum value

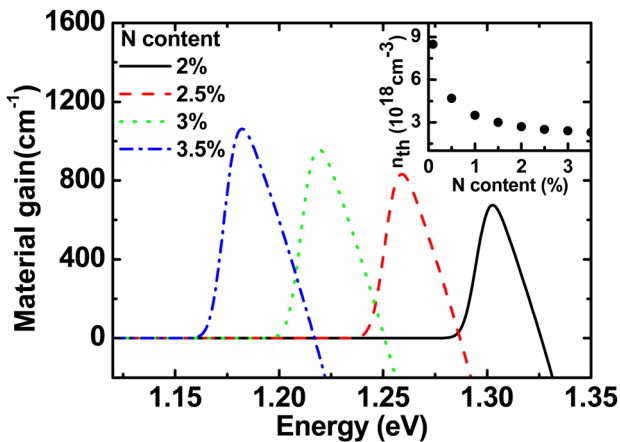


FIG. 4. (Color online) Material gain for TE polarisation at 300 K for a 8 nm thick Ga(N_xAs_{0.92-x}P_{0.08})/GaP QW on GaP substrate for a carrier density of $4 \times 10^{18} \text{ cm}^{-3}$. The band structure is calculated at 0 K and a shift of 50 meV is assumed to get the band structure at 300 K. The inset represents the transparency threshold as a function of N content.

in the $650\text{-}1050 \text{ cm}^{-1}$ range. The discrepancy is probably associated to additional losses for the experimental structure, related to the material itself, like interstitial non radiative N centers or barrier intraband recombinations. Moreover, these calculated gains are similar to those encountered in unstrained InGaAs/InP or GaAs/AlGaAs systems,³² despite the partial N-character of the CB edge which reduces the oscillator strength. This issue is compensated by the CB large effective mass. Nevertheless, this large effective mass may have dramatic consequences on cavity losses of laser structures and on transparency thresholds. The influence of N concentration on the transparency threshold is illustrated in the inset of Fig. 4. The transparency threshold increases dramatically as the N content decreases as a result of CB edge localisation.

In summary, we have used the $sp^3d^5s^*s_N$ TB model to calculate the band structure and the optical gain of strained diluted nitride Ga(NAsP) QWs. The N-related level is found to be located below the conduction band minimum of the GaAsP host material for all the arsenic composition range, giving a N-like character of Ga(NAsP) conduction band edge. This result has large influence on the material gain evolution as a function of the N content.

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