

**Full Potential Calculation of the Band-Gaps in GaP/GaN Superlattices**Noureddine Mehnane,<sup>1,\*</sup> Nabila Oukli,<sup>2,\*</sup> and Hamza Abid<sup>1,\*</sup><sup>1</sup>*Applied Materials Laboratory, Faculty of Technologies,  
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The present paper deals with the electronic properties of GaP and GaN zinc-blende/zinc-blende superlattices using the plane wave version of the full potential linear muffin-tin orbital (FPLMTO) method, which allows an accurate treatment of the interstitial regions. It is found that bowing, which is known to occur for ternary GaPN dilute nitrides, is absent from GaP/GaN “dilute nitride” superlattices with N concentrations greater than 7%, but it can be obtained in these same superlattices for high nitride concentrations.

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**I. INTRODUCTION**

Interest in nitride systems made of both GaP and GaN is mostly due to the properties of these two binaries, but also to the findings concerned with the so called “dilute” nitrides. The latter are a novel set of semiconductor alloys, of interest both from a fundamental perspective and for a wide range of potential applications [1]. Initial interest in dilute nitrides came from two different directions: (i) from the motivation in the 1960s and 1970s to improve the radiative efficiency of GaP-based green LEDs through N doping [2], (ii) and more recently, there has been significant interest in Ga(In)NAs, where replacing As by N leads to a very large band-gap bowing, and a dramatic reduction in the energy gap [3]. Both of these effects are due to the large difference in electronegativity and size between N and the other group V atoms [4].

The fundamental physics of dilute nitride impurities in GaAs and GaP are characterized by the formation of a nitrogen state localized near the bandgap ‘cluster states’ (CS), where the recent works suggest that the properties of the alloys can be analyzed in terms of (i) small nitrogen (CS), and (ii) delocalized perturbed host states (PHS). The CS are ‘deep levels’, due to the differences in atomic size and orbital energies between a nitrogen and the phosphorus atom it substitutes [5]. It is well known that nitrogen (N) incorporation into III-V semiconductor compounds promotes a large band-gap reduction [6].

GaPN represents a novel semiconductor alloy that has attracted considerable interest as a candidate for application as a light emitting diode (LED) [2]. The GaPN alloy has interesting optical properties, such as the presence of a direct transition gap, although

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the host semiconductor GaP is of indirect transition. The optical transition of the GaPN alloy with N composition larger than 0.5% changes from indirect transition ( $\Gamma - X$ ) to direct transition ( $\Gamma - \Gamma$ ) [7]. Replacing a small fraction of phosphorus by nitrogen in GaPN produces states in the band gap close to and just below the host GaP conduction band minimum energy at the  $X$  high symmetry point. The main models used in the literature to describe the evolution of these states are the impurity-band (IB) model [8, 9], the empirical pseudopotential-based model [10], and the two-level band anti-crossing (BAC) model [11, 12]. In the IB model, the N-induced states broaden with increasing N to form a continuum absorption band; this is said to occur involving only the nitrogen states without any explicit interaction with the host conduction band [8, 9]. The empirical pseudopotential model has been used to undertake detailed studies of the band structure, a 512 atom supercell predicted a transition from indirect to direct band gap at a N concentration of  $x = 0.03$  [6]. Experimentally the band structure change was observed at very small nitrogen concentrations of  $x \sim 0.005$  [1].

An anti-crossing model describing the interaction between localized N states and the extended conduction band was introduced by Shan *et al.* [11]. In both cases a strong shift to lower energies of the band gap energy of GaP was predicted, the red shift increasing with an increase of the N content for both alloys. The bandgap energy of dilute nitrides decreases markedly with an increase in the N composition  $x$ , which is called large bandgap bowing [13]. The bandgap bowing of the InGaPN alloy with a direct bandgap was estimated with the band anticrossing (BAC) model, which well explained the experimental bandgap of dilute nitrides [11, 12]. The interaction between the localized N state in a dilute nitride and the energy of a conduction band minimum (CBM) at  $E_C$  of the host semiconductor splits the conduction band into two subbands  $E_{\pm}$ , as described in the following formula:

$$E_{\pm} = \frac{E_C + E_N \pm \sqrt{(E_C - E_N)^2 + 4V^2x}}{2}, \quad (1)$$

where  $E_N$  is the energy of the localized  $N$  state and  $V$  a coupling parameter determined by the strength of coupling between the localized and extended states. The parameter  $E_-$  corresponds to the  $\Gamma$  CBM of the dilute nitride. The  $\Gamma$  values of  $E_N$  and  $V$  of the GaPN are  $E_N = 2.25$  eV and  $V = 2.76$  eV [1]. The CBM  $E_C$  at the point  $\Gamma$  is given as

$$E_C = E_{gIII-V}^{\Gamma} + VBO. \quad (2)$$

The parameter  $E_{gIII-V}^{\Gamma}$  is the bandgap energy of the host III-V semiconductor and  $VBO$  is the unstrained valence band maximum [14]. The initial debate to describe the GaPN CB minimum was mainly polarized between two opposite views. Some authors interpreted the strong redshift of the absorption edge of GaPN in terms of an indirect-to-direct transition in combination with BAC-like behavior [15]. Others favoured a polymorphous model based on multivalley coupling as a unified theory for GaAsN and GaN [5]. However, as shown recently by absorption studies of freestanding GaPN films, neither model provides satisfactory agreement with experiment [8].

It has been shown previously that the distribution of N state energies is crucial for understanding several of the properties of GaAsN alloys [16–19] in which the effect of the

gap reduction is known to occur for small fractions of N, which is similar to what happens for GaPN. Since GaAsN is formed from GaAs and GaN, both having direct bandgaps of 1.42 and 3.4 eV, respectively, one could expect their alloy to cover the visible spectrum which lies between the near infrared and ultraviolet. Indeed, this is not the case. Using the photocurrent method, it has been shown that the gap increases with decreasing N concentration [20]. The most important features observed in  $\text{GaAs}_{1-x}\text{N}_x$  and  $\text{In}_y\text{Ga}_{1-y}\text{As}_{1-x}\text{N}_x$  in the typical nitrogen concentration regime ( $x = 0 : 0.05 - 0.03$ ) are the following: (i) A strong decrease of the band gap and a large, composition dependent band gap bowing, largest at small  $x$  ( $x < 0.01$ ) [11, 21]; (ii) A new composition dependent band edge, called  $E_+$ , which lies 0.4 to 0.8 eV above the conduction band minimum (CBM) (denoted as  $E_-$ ) [22].

While GaPN is attracting all the attention, the GaP/GaN superlattices (SLs) have not received any particular attention. Especially, it has been shown that SL systems can be very useful for theoretical investigation of the bowing phenomenon which occurs in dilute nitrides [23]. The latter are able to help to shed light on this problem even when they are not dilute. The reason for that is that the atomic layers of GaN and GaP in GaP/GaN SLs are (artificially) grown separately and with the desired width for each layer. Hence, all kinds of bonds are easily identified, and one can easily investigate separately their effects and also the effect of each atom (taking into account if it is far or close to the interface, etc.). In this view, it is interesting to study the gap variations of GaP/GaN SLs with N. In both cases: (i) reduction of the band-gap reduction with N or, (ii) linear variation with N can be useful for applications. In the first case, more theoretical investigations must be carried out to see if there are other causes than size effects behind this phenomenon, and in the second case GaPN systems without bowing can be expected to be obtained. Such systems allow one also to study GaPN systems with N atoms incorporated not as a point defect in GaP but (approximately) as a layered defect, like in the above-cited SLs. Therefore, the gap variations with N in these superlattices are our main purpose in the present work.

## II. DETAILS OF THE CALCULATION

We have employed the first principle full potential linear muffin-tin orbital (FPLMTO) method as implemented in the computer code lmtART [24–26]. The exchange correlation energy of electrons is described in the local density approximation (LDA) [27, 28] using the parameterization of Perdew *et al.* [29]. In this method, the unit cell is divided into non-overlapping muffin-tin spheres of radius RMT and an interstitial region. The Kohn-Sham wave functions are expressed in spherical harmonics within the spheres. The MT radii used for the investigated structures are listed in Table I.

Both the LMTO basis set and charge density are expanded in spherical harmonics up to  $l_{\text{max}} = 6$  ( $l_{\text{max}}$  being the maximal angular momentum). We have checked the convergence on the Fourier and mesh division parameters which are involved in the calculations. A k-mesh of  $12 \times 12 \times 12$  and  $36 \times 36 \times 36$  divisions was considered for the fast Fourier transform in all cases.

TABLE I: The MTS radius used for the investigated structures (in atomic units).

	Ga	N	P
GaN	1.980	1.687	—
GaP	2.175	—	2.262
GaP <sub>0.875</sub> N <sub>0.125</sub>	2.139	2.226	2.226
GaP <sub>0.927</sub> N <sub>0.083</sub>	2.154	2.242	2.242
GaP <sub>0.937</sub> N <sub>0.063</sub>	2.159	2.247	2.247
GaP1/GaN1	2.138	1.982	1.982
GaP1/GaN3	2.014	1.742	1.975
GaP2/GaN2	2.071	1.845	2.091
GaP3/GaN1	2.095	2.180	2.180
GaP3/GaN3	2.237	1.937	2.112
GaP4/GaN4	2.111	1.853	2.100
GaP5/GaN1	2.145	2.086	2.186
GaP7/GaN1	2.160	2.106	2.214

For binaries, a primitive cell is considered. Each position contains two atoms, the first one being (Ga) and the second one being (N or P). The second atom is obtained from the first atom by a shift of  $(1/4, 1/4, 1/4)a_0$  in the zinc blende phase,  $a_0$  being the lattice parameter of the binary (GaP or GaN). For the ternary systems, tetragonal elementary cells of 16, 24 and 32 atoms have been considered at  $x = 0.125$ ,  $x = 0.083$ , and  $x = 0.063$ , respectively. On the other hand, we adopted the notation  $SL(m, n)$  for SLs with  $m$  monolayers of GaP and  $n$  monolayers of GaN, each monolayer contains one cation and one anion. As an example, we show in Fig. 1 the direct lattice of a (001) growth axis  $SL(1, 1)$ . The link between the bulk and the SL direct lattices is shown in the figure. In Fig. 2, the reciprocal lattice of  $SL(m, n)$  is represented in a unified manner for all values of  $m$  and  $n$ ,  $m + n$  being even. In the case of a (001)  $SL(m, n)$ , the high symmetry points  $\Gamma$  and  $M$  are identical to  $R$  and  $X$ , respectively.

### III. RESULTS AND DISCUSSIONS

We have calculated the total energy of the zinc blende of all our compounds and superlattices as a function of the volume. The SL systems have the particularity that atoms of different species are ordered in successive atomic planes with chosen periodicity and allow us to control the coupling between atomic orbitals. Hence, the period of our SL is  $D = L \times a_{SL}$  with  $L = (m + n)/2$ ,  $a_{SL}$  being the equilibrium lattice constant of

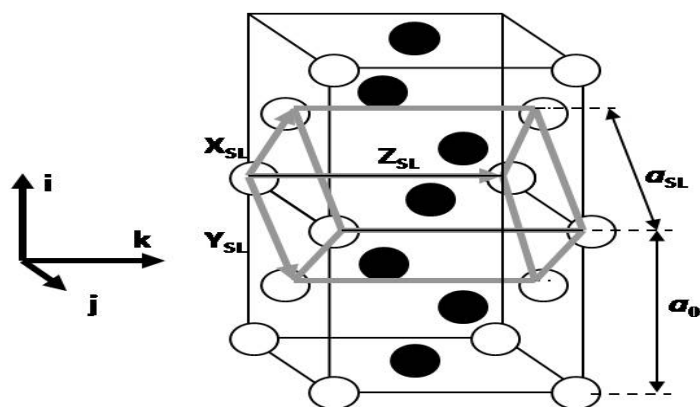


FIG. 1: The direct lattice of a [001] growth axis  $SL(1,1)$ . Its delimitations are shown with bold gray lines. Each monolayer is represented with spherical atoms of a different colour (white and black).

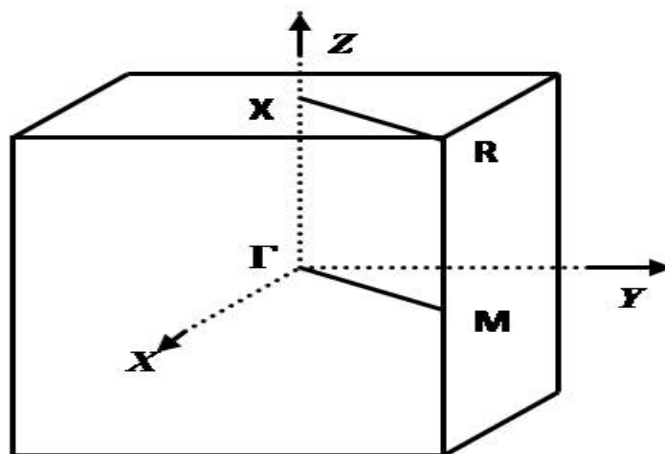


FIG. 2: The Brillouin zone of (001) growth axis  $SL(m,n)$ ,  $m+n$  being even. The high symmetry points  $\Gamma$  and  $M$  are identical to  $R$  and  $X$ , respectively.

the SL in the  $x$  direction. Then, by fitting to the Murnaghan equation of state [30], the equilibrium volume, and the equilibrium lattice constant have been calculated. The results are summarized in Table II. Volume and energy are per single formula unit, which is equal to 2 for binaries, and to  $L$  for SL systems. The calculated equilibrium lattice parameters of our binaries are 4.480 Å and 5.422 Å, which differ by only 0.69% and 0.52% from the experimental values of 4.511 Å for GaN and 5.4505 Å for GaP, respectively [35]. This shows that the method used here is reliable. In all cases, we have checked that the equilibrium

lattice parameter presents in general a linear variation with the GaN proportion in the SL (and the N proportion in ternaries). Thus, the virtual crystal approximation is valid for these cases. Fig. 3 shows for example this variation for the case  $m + n = 4$ .

TABLE II: The structural parameters of all our compounds and superlattices.  $V_0$  is the equilibrium volume,  $a_0$  represents the lattice constant of bulk materials. In the case of a SL,  $a_0$  is shown in Fig. 1 and the link with the SL lattice parameter is obvious: ( $a_0 = \sqrt{2}a_{0,SL}$ ).

	$V_0$ ( $\text{\AA}^3$ )	$a_0$ ( $\text{\AA}$ )	$a_{SL}$ ( $\text{\AA}$ )	$a_0/c_0$
Binaries				
GaN	22.476*	4.480*4.5 <sup>b,c</sup> 4.4614 <sup>f</sup> 4.511 <sup>EXP</sup>	—	1
GaP	39.843*	5.422*5.4505 <sup>c</sup> 5.451 <sup>d</sup> 5.3813 <sup>f</sup> 4505 <sup>EXP</sup>	—	1
The ternary systems				
GaP <sub>0.875</sub> N <sub>0.125</sub>	38.001*	5.335*	—	2
GaP <sub>0.927</sub> N <sub>0.083</sub>	38.792*	5.372*	—	3
GaP <sub>0.937</sub> N <sub>0.063</sub>	39.033*	5.384*	—	4
<i>SL</i> ( $m, n$ ) systems with $m + n = 4$				
GaP <sub>1</sub> /GaN <sub>3</sub>	26.529*	4.732*	3.346*	2.828
GaP <sub>2</sub> /GaN <sub>2</sub>	31.478*	5.010*	3.543*	2.828
GaP <sub>3</sub> /GaN <sub>1</sub>	35.652*	5.223*	3.694*	2.828
<i>SL</i> ( $m, n$ ) systems with $m = n$ (except the case of $m = n = 2$ which is presented above)				
GaP <sub>1</sub> /GaN <sub>1</sub>	31.923*	5.034*	3.560*	1.414
GaP <sub>3</sub> /GaN <sub>3</sub>	36.402*	5.244*	3.719*	4.243
GaP <sub>4</sub> /GaN <sub>4</sub>	31.882*	5.033*	3.559*	5.657
<i>SL</i> ( $m, n$ ) systems with $m = 5, 7$ $n$ is fixed to 1 (except the case of $m = 1, 3$ which is presented above)				
GaP <sub>5</sub> /GaN <sub>1</sub>	37.341*	5.304*	3.751*	4.243
GaP <sub>7</sub> /GaN <sub>1</sub>	38.254*	5.346*	3.781*	5.657

\*Present calculations, <sup>b</sup>Reference [31],

<sup>c</sup>Reference [32], <sup>d</sup>Reference [33],

<sup>f</sup>Reference [34], <sup>EXP</sup>Reference [35].

We have calculated the band structures of both GaP and GaN. The GaN binary compound has a direct band gap, while GaP is an indirect band gap semiconductor with the top of the valence band (VB) at  $\Gamma$  and the bottom of the (CB) both at  $X$ . The values of the  $\Gamma - X$  indirect gap of GaP and of the  $\Gamma - \Gamma$  direct gap of GaN are found to be

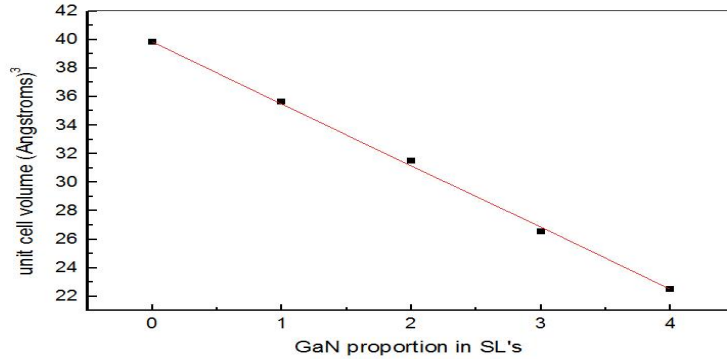


FIG. 3: The unit cell volume as a function of the GaN monolayers and the number of  $SL(m, n)$  in the case of  $m + n = 4$ . The squares represent the calculated unit cell volume and the solid line represents a linear interpolation of the binary

1.518 eV and 1.91 eV, respectively. The calculated direct band gap  $\Gamma - \Gamma$  of GaP is about 1.796 eV. The difference in the indirect band gap in GaP for the present work and the experimental value is 0.742 eV. We recall that gaps are in general underestimated by the LDA, but this will not alter the conclusions of the present work, since they are not related to the quantitative estimation of gaps.

Then, we have calculated the band structures and plotted the gap variations for all our ternary systems of  $\text{GaP}_{1-x}\text{N}_x$  (Fig. 4). One very important remark for the ternaries is that the unit cell considered here for calculations does not represent the primitive cells, so in general the lower gaps obtained here do not represent always the true fundamental gaps (which are obtained with primitive cells). This is due to the fact that when the fundamental gap is indirect for the primitive cell, the zone folding effect which occurs for a multiple cell is able to transform it into a direct gap. However, this fact does not prevent us from giving conclusions about the bowing in these alloys, because the lower gap which occurs in the multiple cell is (in general) linked to the fundamental gap of the primitive cell, except that if it is indirect for the primitive cell, it can become direct in the multiple cell. We remind also that high symmetry points are different in the two kinds of cells. Hence, the bowing effect can be inferred from the multiple cell gap variations.

For our chosen values of  $x$  ( $x = 0.0625, 0.083, \text{ and } 0.125$  in  $\text{GaP}_{1-x}\text{N}_x$ ), which make our compounds to be within the limits of the dilute nitrides, Fig. 4 indicates that there is a clear effect of bowing. The lower gap is the  $\Gamma - M$  gap for  $x = 0.0625$  (6.25%), then it is the  $\Gamma - A$  gap for  $x = 0.083$  (8.3%), and becomes again the  $\Gamma - M$  gap for  $x = 0.125$  (12.5%). The minima of the CB in these three lower gaps are located at  $M$  or at  $A$  and are due to zone folding, the quantum states in these points are linear combinations of two different sets of high symmetry points of the reciprocal lattice of the primitive cells. Hence, from this result we infer that the minimum of the CB of the primitive cell (and so the true fundamental gap) is not located at the same high symmetry point. In fact, both the  $\Gamma - M$  and  $\Gamma - A$  gaps are non-linearly varying,  $\Gamma - M$  ( $\Gamma - A$ ) increases (decreases) then decreases

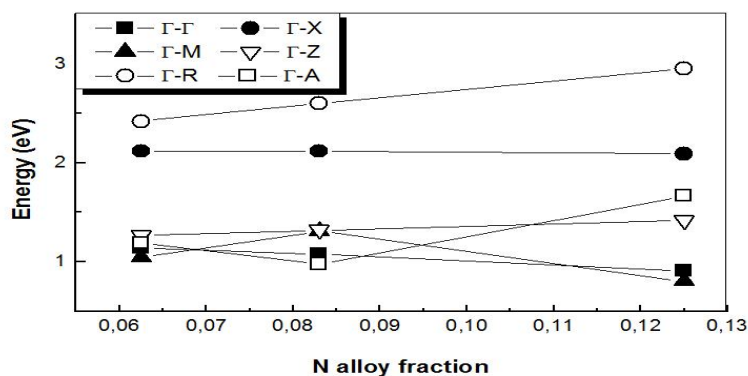
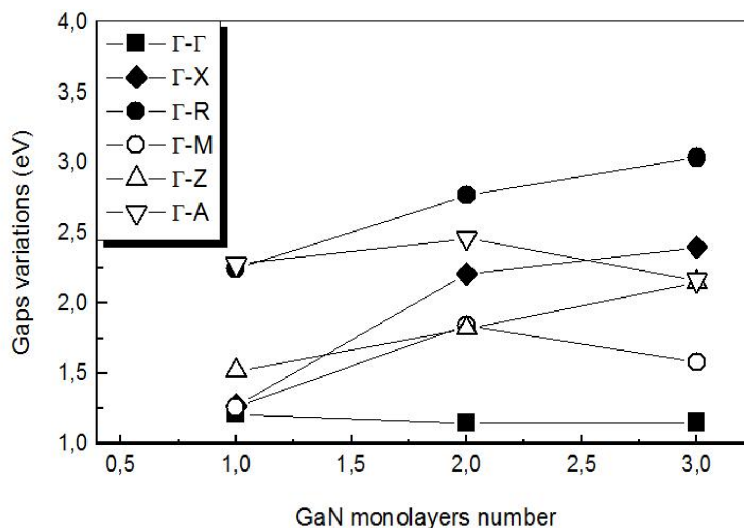


FIG. 4: Gap variations with the N fraction in the alloys.

(increases). Furthermore, it is interesting to note that the  $\Gamma - \Gamma$  gap varies linearly, but is significantly lower than the fundamental gaps of both GaP and GaN (and also lower than the  $\Gamma - \Gamma$  gap of GaP).

Let us now focus on the SLs, for which we recall that we have taken into account the correct primitive cell so that the gaps obtained here are the true ones. An interesting feature is obtained in the present SLs, the GaP/GaN systems constituted from both indirect and direct bandgap bulk materials are found to have a direct bandgap. To investigate this phenomenon, we have calculated the band structures of  $SL(m, n)$  at their respective equilibrium volumes for a different number of monolayers  $m$  and  $n$  with  $m + n = 4$ , then we have plotted the gap variations for all of them (Fig. 5).

FIG. 5: Gap variations with the GaN monolayer numbers of  $SL(m, n)$  in the case of  $m + n = 4$ .

We remind the reader that the SL high-symmetry points do not have the same mean-



ing in binaries and ternaries, except for  $\Gamma - \Gamma$ . We remark that for all our systems the fundamental gap remains direct with both the top of the (VB) and the bottom of the (CB) located at  $\Gamma$ . It is clear that for  $n = 1$ , the  $\Gamma - X$  and  $\Gamma - M$  gaps are very close to the  $\Gamma - \Gamma$  gap (but remain greater than the  $\Gamma - \Gamma$  gap), this is due to the zone-folding effect which occurs in the Brillouin zone when passing from the bulk to the SL, the quantum states at each reciprocal wavevector of the SL being formed from quantum states of selected sets of reciprocal wavevectors of bulk binaries. The zone-folding does not have the same effect for all values of  $n$ . Going from one monolayer to three monolayers of GaN in the SL (Fig. 5), we remark that the fundamental  $\Gamma - \Gamma$  direct gap remains approximately constant. We remark also that this  $\Gamma - \Gamma$  direct gap is lower than the fundamental gaps of both GaP ( $\Gamma - X$ ) and GaN ( $\Gamma - \Gamma$ ), and thus is not obtained from their interpolation. Here, the fundamental gap of GaP is very important, because the minimum of the CB of GaP is located at the high symmetry point X, which folds for  $m + n$  even to the point  $\Gamma$  of the SL. So, since the  $\Gamma - \Gamma$  direct gap of our SLs is not a “mean” value of the gaps of GaP and GaN, can we conclude from this fact that we have bowing? It seems to us that for SLs the answer cannot be given at this stage, and more care must be taken for two reasons: (i) the magnitudes of the  $\Gamma - \Gamma$  gaps of the SLs were less different from the fundamental gaps of binaries than the  $\Gamma - \Gamma$  gaps of ternaries, so we can expect other effects to be behind this difference, and (ii) the fundamental gap remains located at  $\Gamma$ , so that the other high symmetry points do not help us to a conclusion on the gap bowing.

So, in order to be able to make a conclusion about the gap bowing in SLs, we propose to investigate what could be the impact of the incorporation of small amounts of nitrogen (i.e., of a small number of GaN monolayers). Thus, we have investigated  $(\text{GaP})_m/(\text{GaN})_n$  superlattices for different numbers of monolayers  $m$  with  $m = 1, 3, 5, 7$  and  $n = 1$  (i.e., the total number of monolayers varies from 2 to 8). We remark that the fundamental gap remains direct, with both the top of the VB and the bottom of the CB located at  $\Gamma$  (Fig. 6). Even if there is a competition between  $\Gamma - \Gamma$ ,  $\Gamma - M$ , and  $\Gamma - R$ , the fundamental gap remains at  $\Gamma - \Gamma$ , and the latter is increasing from  $SL(m = 1, n = 1)$  to  $SL(m = 5, n = 1)$  then it becomes stable and close to the GaP indirect fundamental gap  $\Gamma - X$ . However, since we go from  $m = 1$  to  $m = 7$  (with the number of GaN monolayers constant  $n = 1$ ), so we are going from a thin  $SL(m = 1, n = 1)$  to what we can call a “dilute”  $SL(m = 7, n = 1)$ , in which we have approximately 7% of N atoms only with 93% represented by Ga and P atoms. Fig. 6 shows no anomalous variation of the  $\Gamma - \Gamma$  gap, which becomes stable after  $m = 3$ . Thus, no gap bowing is detected in our SL systems and we are encouraged to conclude that gap bowing in GaP/GaN SLs does not occur at N concentrations above 7%. Gap bowing at concentrations lower than 7% has not been investigated in this work.

In what follows, we are going to show what we have obtained when we have calculated the band structures of our SLs for  $m = n = 1, 2, 3, 4$  (i.e.,  $m + n = 2$  to 8), in their respective equilibrium volumes. In all cases, the fundamental gap remains direct, with both the top of the VB and the bottom of the CB located at  $\Gamma$  (Fig. 7). For  $n = 1$ , the  $\Gamma - M$  and  $\Gamma - R$  of the SLs are in competition with the  $\Gamma - \Gamma$  gap. We remark that the  $\Gamma - \Gamma$  gap increases with thickness from  $m = n = 1$  to  $m = n = 2$  by 0.353 eV, and when  $n$  increases, the  $\Gamma - \Gamma$  gap becomes smaller: it decreases from  $m = n = 2$  to  $m = n = 4$  by 1.013 eV. The same

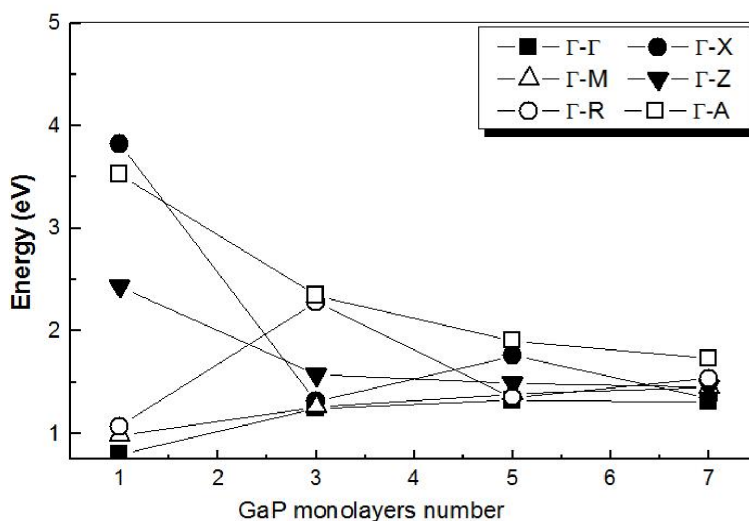


FIG. 6: Variation of the transition energies versus the number  $m$  of monolayers in the superlattice  $(\text{GaP})_m/(\text{GaN})_n$  ( $n$  is fixed to 1).

remark holds in the case of the  $\Gamma - M$  gap which follows similar variations. In the case of  $\Gamma - R$ , we note that the gap increases drastically from  $m = n = 1$  to  $m = n = 3$ , and decreases more for  $m = n = 4$ , for which this gap reaches a value very far from the mean value of the GaP and GaN relative gaps. The  $\Gamma - \Gamma$  gap is the reverse to that observed in both the preceding cases. This finding shows that gap bowing is present but not for “dilute” SLs. If we compare the magnitudes of the  $\Gamma - \Gamma$  gap in  $SL(m = 7, n = 1)$  and  $SL(m = 4, n = 4)$ , both having  $m + n = 8$ , we conclude that the bowing effect is present for the second case  $SL(m = 4, n = 4)$ , for which we have 25% of N atoms, and not the first case  $SL(m = 7, n = 1)$ , for which we have only 7% of N atoms.

#### IV. CONCLUSION

In summary, we presented an ab-initio calculation of the structural and electronic properties of the cubic and tetragonal Ga(P,N) alloys and  $(\text{GaP})_m/(\text{GaN})_n$  SLs using the PLW-FPLMTO method. Our results show that bowing which occurs in dilute ternary nitrides does not occur in the same way in GaP/GaN SLs. In SLs, this bowing appears at for example 25% of N concentration, but seems to be absent in the case of “dilute” nitride SLs at 7% of N concentration.

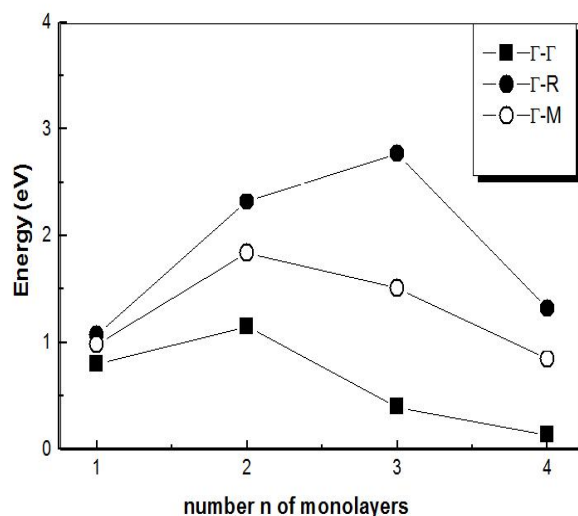


FIG. 7: Gap variations versus the number  $n$  of monolayers of  $SL(n, n)$  superlattices.

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