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First Principles Investigation of Structural and Electronic Properties of AlN/GaN Superlattices Growth Along Various Crystallographic Axes

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Introduction

The group III-nitrides semiconductors, InN, GaN and AlNand their alloys are of continuing great interest due to their vast technical application as design of Laser Diodes and Light- Emitting Diodes (LED's) operating in the short-wavelength from blue–green [1-5], ranging from 0.667 to 4.904 eV. The AlN and GaN lattice parameters are approaching each other, and significantly smaller than that of InN [6], the challenge of the lattice mismatchbetween the epitaxial layers and substrates can be solved by introduced a small amount of InN [7].

While AlGaN is attracting all the attention, the AlN/GaN SL's with various growth axis directions have notreceived a particular attention. Especially, it has been shown that SL systems can be very useful for theoretical investigation to the determination of their electronic properties. The reason for that is that atomic layers of GaN and AlN in AlN/GaN SL's are (artificially) grown separately and with the desired width for each layer

Theoretical Study

For binaries, a primitive cell is considered. Each position contains two atoms, the first one being (Ga or Al) and the second one being (N). 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 (AlN or GaN). The investigated structures consist of idealquantum well superlattices made of a periodic sequence of monolayers of AlN and monolayers of GaN. On the other hand, we adopted the notation $SL(m,n)$ for SL's with$m$ monolayers of AlN and n monolayers of GaN, each monolayer contains one cation and one anion. We consider the SLs with the growth axis along the three directions. We restrict ourselves to the case for which $(m+ n)$ is even.

Results and Discussion

We have calculated the band structures of both binaries AlN and GaN. That is, the valence band (VB) maximum and conduction band (CB) minimum are found at the Γ point. Comparison with previous experimental results reveals that the present calculated bandgaps of 3.406 eV for AlN and 1.916 eV for GaN are underestimated compared to the experimental values of 6.28 eV for AlN and 3.20 eV for GaN [35], but this will not alter theconclusions of the present work since they are not related to the quantitative estimation of gaps.

For the growth axis (001), the high symmetry points B and Y do not exist in the (001), because in

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this case, they are identical to *R* and *X* respectively. Thus, we have just represented *R* and *X* but we labelled them *B* and *Y* to allow comparison. In all cases, the gap remains directly with the top of VB and the bottom of CB both at □ and is about 2.495 eV with *m* = *n* = 3. However, we remark that the *Γ*–*Γ* gap decreases with thickness from *m* = *n* = 1 to *m*= *n* = 2 by 0.084 eV, and when *n* increases, the *Γ*–*Γ* gap becomes smaller: it decreases from *m* = *n* = 2 to *m* = *n* = 3by 0.112 eV. The same remark holds in the case of the *Γ*– *X, Γ*–*M, Γ* –*Z* and *Γ*–*A* gap which follows similar variations (but remain greater than the *Γ*–*Γ* gap). In the case of *Γ* – *R*, we note that the gap increases from *m* = *n*= 1 to *m* = *n* = 2, and decreases more for *m* = *n* = 3. We remark also that this *Γ*–*Γ* direct gap is lower than the fundamental gaps of AlN, and thus is not obtained from interpolation of both parents AlN and GaN.

An interesting feature is obtained in the SLs from (110) and (111) growth axis is found to have a indirect bandgap with *m* = *n* = 1, 2, 3, the top of the valence band (VB) being at *Y* from (110) SL and *R* from (111) SL and the bottom of the CB located at *Γ* and *Z* respectively. When *m*= *n* = 3 the indirect bandgap for the (110) SLs is about 2.437 eV which is close to the direct *Γ*–*Γ* bandgap of 2.453 eV. However, the indirect bandgap for the (111) SLs is about 0.386 eV (an *Γ*–*Γ* bandgap of 0.576 eV), where it shifts towards lower energy when compared to both directions (001) and (110) SLs. Furthermore, the *Y*–*Γ* and *R* –*Z* gaps decreases with thickness from *m* = *n* = 1 to *m* = *n* = 3 by 0.254 eV and 0.042 eV from (110) and (111)growth axis. We notice also significant changes in the CB behaviour near *M*, *A* and *X* become non-linearly varying, Γ-*M* and Γ-*A* (Γ-*X*) increases (decreases) than decreases (increases) for (110) compared with (001).

Conclusion

The most important results are that all these systemsexhibit direct or indirect band gap, and that (AlN)*n*/(GaN)*n* superlattices are energetically more stablewith increasing *n*. However, it is shown that the band structures of (001) is different from (110) and (111) SL's. We believe that a larger influence of *sp* and *pd* coupling between Ga and N atoms modify the nature of the gap andreduce here value.

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